FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

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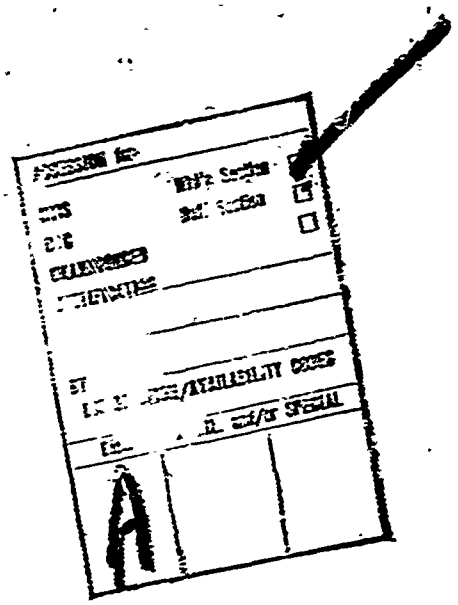

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FOREWORD

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This technical report has been reviewed and is approved.

Paul J. Daily, Col. USAF
Chief, Technology Division

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A fast computer program for predicting nonequilibrium rocket plume properties is described. The analytical model assumes parallel turbulent (or laminar) mixing between concentric chemically reacting streams and can also be used for studying chemical lasers and re-entry wakes. The equations for free shear layer mixing with nonequilibrium chemistry are solved via a mixed implicit/explicit finite difference scheme which efficiently predicts flow properties and composition, even when many chemical reactions are near equilibrium. The stability problems inherent in fully explicit finite difference schemes are shown to be eliminated, and stable integration step sizes are shown to be increased by up to 4 orders of magnitude. Computer run times for typical afterburning rocket plume calculations are shown to be decreased by more than one order of magnitude over the original (fully explicit) AeroChemaxisymmetric mixing with nonequilibrium chemistry program. Both the analysis and computer program write-up are presented, including a sample calculation and a FORTRAN listing.

NOMENCLATURE

a	defined by Eq. (15b)
$a_{\frac{1}{2}}$	defined by Eq. (33)
a'	attenuation per unit length
A	constant in expression for k_f (see Eq. (23))
$b_{\frac{1}{2}}$	defined under Eq. (25b)
B	activation energy (see Eq. (23))
c_p	specific heat of mixture ($\sum_i X_i c_{p_i}$)
c_{p_i}	specific heat of ith species
e	electronic charge
F_i	defined as X_i/W (= Y_i/W_i)
FDL	factor used for the external control of integration step size
g_i	Gibbs free energy of ith species at standard state (1 atm)
ΔG	change in standard Gibbs free energy for a reaction, $\sum_i (g_i)_{\text{products}} - \sum_i (g_i)_{\text{reactants}}$
h	enthalpy of mixture
h_i	enthalpy of ith species
h_{298_i}	heat of formation of ith species at T = 298 K
k_f	forward rate coefficient
K	eddy viscosity coefficient (see Section VI)
$\bar{K}$	eddy viscosity coefficient for Donaldson/Gray model (see Eq. (32))
K_p	equilibrium constant
Le	Lewis number (laminar or turbulent)
m_e	electron mass
$M_{\frac{1}{2}}$	Mach number at half radius, defined under Eq. (32)
N	temperature exponent in reaction rate equation (Eq. (23))
n_e	electron density
Q	arbitrary dependent variable (see Eqs. (13) - (15))

Q_e	electron-neutral collision cross section
p	static pressure
Pr	Prandtl number (laminar or turbulent)
r	coordinate normal to jet centerline
r_i	inner mixing zone radius
r_j	jet radius
$r_{\frac{1}{2}}$	defined under Eq. (28b)
$\overline{r}_{\frac{1}{2}}$	defined under Eq. (27)
R	universal gas constant
T	static temperature
u	x component of velocity
v	r component of veclocity
v_e	electron velocity
$\dot{w}_i$	molar rate of production of ith species
$\dot{w}^{(j)}$	molar rate of production from jth reaction
W	molecular weight of mixture $(\sum_i F_i)^{-1}$
W_i	molecular weight of ith species
x	coordinate parallel to jet centerline
Δx	$x_{n+1} - x_n$
X_i	mole fraction of ith species
Y_i	mass fraction of ith species

Greek

α	constant for external control of eddy viscosity (see Eqs. (25) - (31))
$\Delta\Psi$	$\psi_{m+1} - \psi_m$
ϵ	eddy diffusivity for turbulent flow; defined as μ/ρ
η	defined by Eq. (25)
μ	viscosity (or eddy viscosity for turbulent flow)
ν_e	electron-neutral collision frequency
ρ	density
σ	electrical conductivity

Ψ	stream function
ω	signal frequency

Subscripts

e	evaluated at edge of mixing layer (free stream)
e^-	electrons
i	ith species
j	value at nozzle (jet) exit
m	Ψ index in grid network
n	x index in grid network
o	evaluated at axis of symmetry, r = 0

Miscellaneous

$\lvert\ \rvert$	absolute value
$\left(\frac{\partial}{\partial \beta}\right)_\gamma$	partial derivative with respect to β; γ being held constant
$\sum_i$	summation over i species

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I. INTRODUCTION

The need to accurately determine electromagnetic wave/plume interactions[1,2] has motivated the development of several programs[3-6] to predict the electrical properties of turbulent rocket exhaust plumes.* Each program uses the same gas dynamic model (parallel mixing between two concentric streams), but only the AeroChem program of Mikatarian and Pergament accounts for nonequilibrium chemistry effects; the others[3-5] assume local thermochemical equilibrium to prevail. Attempts to account for transverse radar attenuation data (taken with focused microwaves) under simulated altitude conditions using equilibrium chemistry programs generally fail. Indeed, it has been demonstrated by Pergament and Jensen[7,8] that finite-rate chemical kinetics must be incorporated into rocket plume calculations to accurately predict plume temperatures, electrical properties, etc.

Conceptually the numerical solution of the equations describing axisymmetric mixing with nonequilibrium chemistry presents few difficulties. A fully explicit finite difference scheme[4] yields an accurate solution to the problem. Unfortunately, however, on many occasions the stability requirements associated with the explicit integration scheme are found to so severely limit maximum step sizes (e.g. on the order of 10^{-5} to 10^{-10} ft) that computer solutions become economically prohibitive.† This "stiffness" in the equations,[9,10] (which results in small step sizes) is found to be restricted to nonequilibrium flows where one or more of the chemical reactions is at or near-equilibrium, a situation typical of relatively low altitude ($< \approx 70$ kft) afterburning plumes.

In this computer program we utilize a new numerical technique to solve the partial differential equations (in finite-difference form) describing turbulent (or laminar) shear flows with nonequilibrium chemistry: Implicit differences are used in the solution of the species conservation equations‡

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*References 3 and 5 are unclassified descriptions of the solution techniques used in the Naval Weapons Center and Lockheed Propulsion Company codes. Further information on these codes may be found in the classified literature.

†For frozen (non-reactive) flow the governing equations can be integrated quite rapidly using explicit differences.

‡This appears to be the first program to utilize implicit differences for free shear layers with nonequilibrium chemistry, although such schemes have been applied to one-dimensional nonequilibrium nozzle flows.[11,12]

and explicit differences are used for the momentum and energy equations. This mixed implicit/explicit scheme eliminates the instability problems which characterize fully explicit schemes and allows integration step sizes to be increased by orders of magnitude without sacrificing accuracy. Those rocket exhaust plume predictions which could not be made with the original AeroChem program[4] (which uses the fully explicit scheme) because the stable step size approached 10^{-10} ft, are quite easily handled by the new program. Most importantly, for the more typical case in which average step sizes range from 10^{-4} to 10^{-2} ft, the new program reduced computer run times by at least an order of magnitude. (A detailed comparison between rocket plume calculations using the original fully explicit difference scheme and the new mixed implicit/explicit scheme is given in Appendix D.)

The gas dynamic model assumes parallel mixing between the rocket exhaust products and surrounding air (either quiescent or moving), and allows for non-uniform initial conditions at the nozzle exit plane.* Lewis and Prandtl numbers are assumed to be constant, and pressure is allowed to vary parallel to the plume axis. Turbulent transport is described via an appropriate eddy viscosity model and Sutherland's law is used to calculate the viscosity for laminar flow. The program is quite general; it allows any chemical reaction mechanism (and associated rate coefficients) to be used as long as thermodynamic data are available for all species. Thermodynamic data, taken directly from the JANNAF Tables, are input in tabular form.

This report gives the governing partial differential equations and their finite difference formulations, the various eddy viscosity models which may be input to the program, a description of the input data, the output from a sample calculation and a complete FORTRAN listing. The computer output gives detailed axial and radial distributions of velocity, temperature, density and species mole fractions. These results are used to calculate electron densities and electron-neutral collision frequencies which, in turn, are used to determine radar attenuation transverse to the plume and electrical conductivity.

Although the program was written in response to a need for fast predictions of relatively low altitude afterburning rocket plume electrical properties, it can equally well be used for applications to missile base heating and IR radiation problems.

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*Thus it is possible to account for the effects of an initial boundary layer on the properties in the mixing region.

II. GOVERNING EQUATIONS

A. Conservation Equations and Boundary Conditions

The following equations describe the free-shear layer turbulent or laminar mixing of co-flowing axisymmetric streams undergoing chemical reactions. For turbulent flow all properties are interpreted to be the mean (time-averaged) values. The eddy viscosity, μ, is then described by one of the phenomenological expressions given in Section VI.

Global Continuity

$$\frac{\partial}{\partial x}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(\rho v r) = 0 \tag{1}$$

Conservation of Species

$$\rho u \frac{\partial F_i}{\partial x} + \rho v \frac{\partial F_i}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{Le}{Pr}\,\mu r \frac{\partial F_i}{\partial r}\right) + \dot{w}_i \tag{2}$$

Conservation of Momentum

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} = -\frac{dp}{dx} + \frac{1}{r}\frac{\partial}{\partial r}\left(\mu r \frac{\partial u}{\partial r}\right) \tag{3}$$

Conservation of Energy

$$\rho c_p \left[u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial r}\right] = u\frac{dp}{dx} + \mu\left(\frac{\partial u}{\partial r}\right)^2 + \frac{1}{r}\frac{\partial}{\partial r}\left[\frac{c_p}{Pr}\mu r \frac{\partial T}{\partial r}\right] + \mu\frac{Le}{Pr}\frac{\partial T}{\partial r}\sum_i c_{p_i}\frac{\partial F_i}{\partial r} - \sum_i \dot{w}_i h_i \tag{4}$$

State

$$\rho = \frac{pW}{RT} \tag{5}$$

The conservation equations are solved subject to the following initial and boundary conditions:

$$\begin{aligned} x = 0: &\quad u = u(r), \; F_i = F_i(r), \; T = T(r) \\ r = 0: &\quad \frac{\partial u}{\partial r} = \frac{\partial T}{\partial r} = \frac{\partial F_i}{\partial r} = 0 \\ r \to \infty: &\quad u \to u_e, \; F_i \to (F_i)_e, \; T \to T_e \end{aligned} \tag{6}$$

Pressure is allowed to vary in the axial direction according to,

$$p = c_0 + c_1 x + c_2 x^2 + c_3 x^3 \tag{7}$$

where c_0, c_1, c_2 and c_3 are input coefficients (Card 5, Cols. 21-60).

B. Transformation to Stream Function Coordinates

It is convenient to transform the equations into a streamline coordinate system and utilize the stream function, Ψ, as the radial coordinate. The transformation from cartesian (x, r) coordinates to streamline (x, Ψ) coordinates (which automatically satisfies global continuity, Eq. (1)) is defined by:

$$\Psi \frac{\partial \Psi}{\partial r} = \rho u r \tag{8a}$$

$$\Psi \frac{\partial \Psi}{\partial x} = -\rho v r \tag{8b}$$

From Eqs. (8a) and (8b) we obtain,

$$\left(\frac{\partial}{\partial r}\right)_x = \frac{\rho u r}{\Psi} \left(\frac{\partial}{\partial \Psi}\right)_x \tag{9a}$$

$$\left(\frac{\partial}{\partial x}\right)_r = \left(\frac{\partial}{\partial x}\right)_\Psi - \frac{\rho v r}{\Psi} \left(\frac{\partial}{\partial \Psi}\right)_x \tag{9b}$$

Introducing Eqs. (9a) and (9b) into Eqs. (2), (3), and (4), gives:

Species

$$\frac{\partial F_i}{\partial x} = \frac{1}{\bar{\Psi}} \frac{\partial}{\partial \bar{\Psi}} \left[\left(\frac{Le}{Pr} \right) \frac{\mu \rho u r^2}{\bar{\Psi}} \frac{\partial F_i}{\partial \bar{\Psi}} \right] + \frac{\dot{w}_i}{m\dot{p}} \tag{10a}$$

and, on the axis of symmetry, $r = \bar{\Psi} = 0$

$$\frac{\partial F_i}{\partial x} = 2\mu \left(\frac{Le}{Pr} \right) \frac{\partial^2 F_i}{\partial \bar{\Psi}^2} + \frac{\dot{w}_i}{m\dot{p}} \tag{10b}$$

Momentum

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u} \frac{dp}{dx} + \frac{1}{\bar{\Psi}} \frac{\partial}{\partial \bar{\Psi}} \left[\frac{\mu \rho u r^2}{\bar{\Psi}} \frac{\partial u}{\partial \bar{\Psi}} \right] \tag{11a}$$

and, on the axis of symmetry, $r = \bar{\Psi} = 0$

$$\frac{\partial u}{\partial x} = -\frac{1}{\rho u} \frac{dp}{dx} + 2\mu \frac{\partial^2 u}{\partial \bar{\Psi}^2} \tag{11b}$$

Energy

$$c_p \frac{\partial T}{\partial x} = \frac{1}{\rho} \frac{dp}{dx} - \frac{1}{\rho u} \sum_i h_i \dot{w}_i + \frac{1}{\bar{\Psi}} \frac{\partial}{\partial \bar{\Psi}} \left[\frac{c_p}{Pr} \frac{\mu \rho u r^2}{\bar{\Psi}} \frac{\partial T}{\partial \bar{\Psi}} \right] + \frac{\mu \rho u r^2}{\bar{\Psi}^2} \left[\left(\frac{\partial u}{\partial \bar{\Psi}} \right)^2 + \frac{Le}{Pr} \frac{\partial T}{\partial \bar{\Psi}} \sum_i c_{p_i} \frac{\partial F_i}{\partial \bar{\Psi}} \right] \tag{12a}$$

and, on the axis of symmetry, $r = \bar{\Psi} = 0$

$$c_p \frac{\partial T}{\partial x} = \frac{1}{\rho} \frac{dp}{dx} + 2\mu \left(\frac{c_p}{Pr} \right) \frac{\partial^2 T}{\partial \bar{\Psi}^2} - \frac{1}{\rho u} \sum_i h_i \dot{w}_i \tag{12b}$$

C. Finite-Difference Formulation

The governing set of parabolic partial differential equations, (Eqs. (10), (11) and (12)), are first rewritten in finite difference form and then solved using a forward marching technique. The chemistry terms, $\dot{w}_n$, in the species continuity equations are evaluated via implicit-differences; the diffusion terms in the species continuity equations and the complete energy and momentum equations are evaluated via explicit-differences. The following finite-difference formulations[13] are used:

$$\left(\frac{\partial Q}{\partial x}\right)_{n+1,\,m} = \frac{Q_{n+1,\,m} - Q_{n,\,m}}{\Delta x} \tag{13}$$

$$\left(\frac{\partial Q}{\partial \bar{\Psi}}\right)_{n,\,m} = \frac{Q_{n,\,m+1} - Q_{n,\,m-1}}{2\Delta\bar{\Psi}} \tag{14a}$$

$$\left[\frac{\partial}{\partial \bar{\Psi}}\left(a\frac{\partial Q}{\partial \bar{\Psi}}\right)\right]_{n,\,m} = \frac{a_{n,\,m+\frac{1}{2}}\left[Q_{n,\,m+1} - Q_{n,\,m}\right]}{(\Delta\bar{\Psi})^2} \tag{14b}$$

$$- \frac{a_{n,\,m-\frac{1}{2}}\left[Q_{n,\,m} - Q_{n,\,m-1}\right]}{(\Delta\bar{\Psi})^2}$$

where

$$a_{n,\,m\pm\frac{1}{2}} = \frac{a_{n,\,m} + a_{n,\,m\pm1}}{2} \tag{15a}$$

and

$$a = \frac{\mu\rho u r^2}{\Psi} \tag{15b}$$

The difference equations that result from applying Eqs. (13), (14) and (15) to Eqs. (10), (11) and (12) are:

Species

$$(F_i)_{n+1,m} - (\bar{w}_i)_{n+1,m}\,\Delta x/(\rho u)_{n,m}$$

$$= \frac{\Delta x}{m(\Delta\Psi)^3}\left\{\left(\frac{Le}{Pr}a\right)_{n,\,m+\frac{1}{2}}\left[(F_i)_{n,\,m+1} - (F_i)_{n,\,m}\right]\right.$$

$$+ \left(\frac{Le}{Pr}a\right)_{n,\,m-\frac{1}{2}}\left[(F_i)_{n,\,m-1} - (F_i)_{n,\,m}\right]\Bigg\} \qquad (16a)$$

$$+ (F_i)_{n,m}$$

and, on the axis of symmetry (m = 0),

$$(F_i)_{n+1,0} - (\bar{w}_i)_{n+1,0}\Delta x/(\rho u)_{n,0}$$

$$= \frac{4\Delta x}{(\Delta\Psi)^2}\left(\frac{aLe}{Pr}\right)_{n,0}\left[(F_i)_{n,1} - (F_i)_{n,0}\right] \qquad (16b)$$

$$+ (F_i)_{n,0}$$

Momentum

$$u_{n+1,m} = \frac{\Delta x}{m(\Delta\Psi)^3}\left\{a_{n,\,m+\frac{1}{2}}\left[u_{n,m+1} - u_{n,m}\right]\right.$$

$$+ a_{n,\,m-\frac{1}{2}}\left[u_{n,m-1} - u_{n,m}\right]\Bigg\} - \frac{\Delta x}{(\rho u)_{n,m}}\left(\frac{dp}{dx}\right)_{n+1,} + u_{n,m} \qquad (17a)$$

and, on the axis of symmetry, $m = 0$

$$u_{n+1,0} = -\frac{\Delta x}{(\rho u)_{n,0}} \left(\frac{dp}{dx}\right)_{n+1} + \frac{4\mu_{n,0}\Delta x}{(\Delta\Psi)^2} \left[u_{n,1} - u_{n,0}\right] + u_{n,0} \tag{17b}$$

Energy

$$T_{n+1,m} = \frac{\Delta x}{(\rho c_p)_{n,m}} \left(\frac{dp}{dx}\right)_{n+1} + \frac{\Delta x}{4m(\Delta\Psi)^3} \left(\frac{\mu}{c_p}\right)_{n,m} \left(u_{n,m+1} - u_{n,m-1}\right)^2$$

$$+ \frac{\Delta x}{m(\Delta\Psi)^3 (c_p)_{n,m}} \left\{ \left(\frac{c_p}{Pr}\mu\right)_{n,m+\frac{1}{2}} \left(T_{n,m+1} - T_{n,m}\right) \right.$$

$$+ \left(\frac{c_p}{Pr}\mu\right)_{n,m-\frac{1}{2}} \left(T_{n,m-1} - T_{n,m}\right) + \frac{1}{4}\left(\frac{1-\mu}{Pr}\mu\right)_{n,m-1} \sum_i (c_{p_i})_{n,m}$$

$$\left. \left(Fi_{n,m+1} - Fi_{n,m-1}\right) \left[T_{n,m+1} - T_{n,m-1}\right] \right\}$$

$$+ T_{n,m} - \frac{1}{(\rho u)_{n,m}} \sum_i (h_i \dot{w}_i)_{n,m} \tag{18a}$$

and, on the axis of symmetry, $m = 0$

$$T_{n+1,0} = \frac{\Delta x}{(\rho c_p)_{n,0}} \left(\frac{dp}{dx}\right)_{n+1} + \frac{4\Delta x}{(\Delta\Psi)^2} \left(\frac{\mu}{Pr}\right)_{n,0} \left[T_{n,1} - T_{n,0}\right] + T_{n,0} - \frac{1}{(\rho u)_{n,0}} \sum_i (h_i \dot{w}_i)_{n,0} \tag{18b}$$

The species mole fractions at station n+1, m are determined from the species conservation equations by linearizing the chemistry terms* (i.e. $(\dot{w}_i)_{n+1,m}$) and inverting the resulting matrix. The linearizations involving species F_i and F_j (for a two-body reaction) or F_i, F_j and F_k (for a three-body reaction) at station n+1 (all variables are known at station n), are given by

$$(F_iF_j)_{n+1} = (F_iF_j)_n + F_{jn}\left[(F_i)_{n+1} - (F_i)_n\right] + F_{in}\left[(F_j)_{n+1} - (F_j)_n\right]$$

$$= -\underline{\underline{(F_iF_j)_n}} + \underline{(F_j)_n}(F_i)_{n+1} + \underline{(F_i)_n}(F_j)_{n+1} \tag{19}$$

$$(F_iF_jF_k)_{n+1} = -\underline{\underline{2(F_iF_jF_k)_n}} + \underline{(F_jF_k)_n}(F_i)_{n+1} + \underline{(F_iF_k)_n}(F_j)_{n+1}$$

$$+ \underline{(F_iF_j)_n}(F_k)_{n+1}. \tag{20}$$

The terms underscored by a single line contribute to the elements of the coefficient matrix, while the terms underscored by a double line contribute to the known column matrix on the right hand side of the matrix equation for the linearized system. Thus the matrix equation takes the form (for N species),

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & & a_{1N} \\ a_{21} & & & & \\ & & & & \\ & & & & \\ a_{N1} & & & & a_{NN} \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ \\ \\ F_N \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ \\ \\ Q_N \end{bmatrix} \tag{21}$$

*The chemistry term does not make the energy equation "stiff"; thus when solving for temperature the chemistry term is treated explicitly.

III. SOLUTION OF FINITE DIFFERENCE EQUATIONS

A. Integration Step Size

An exact stability relationship governing the maximum allowable integration step size, $(\Delta x)_{max}$, cannot be obtained due to the nonlinearity of the governing equations. Instead the step-size requirement to satisfy stability can only be estimated. Following Von Neuman[24] a limit is placed on $(\Delta x)_{max}$ such that all dependent variables (u, T, F_i) always remain equal to or greater than zero. Thus the maximum step size at each radial grid point ($m \neq 0$) as established from the species conservation equation* is estimated to be

$$(\Delta x)_{max} = \frac{m\,(\Delta\Psi)^2}{\left[\frac{Le}{Pr}a\right]_{n,\,m+\frac{1}{2}} + \left[\frac{Le}{Pr}a\right]_{n,\,m-\frac{1}{2}}} \text{ FDL} \qquad (22a)$$

and on the axis, ($m = 0$),

$$(\Delta x)_{max} = \frac{(\Delta\Psi)^2\,Pr}{4\,Le\,\mu} \text{ FDL} \qquad (22b)$$

The actual integration step size, Δx, is taken to be $\frac{1}{3}$ of the smallest value of $(\Delta x)_{max}$ as computed from Eqs. (22a) and (22b). This fraction ($\frac{1}{3}$) was selected on the basis of many trial calculations. Since Eqs. (22a) and (22b) are only approximate an additional factor, FDL, has been incorporated into the program in order to maintain external control (Card 5, Cols. 11-20) on Δx in case smaller step sizes are required to maintain stability of the solution. In addition, the step size can never exceed the input print increment (Card 4, Cols. 21-30).

Should the computed species mole fraction at any radial point become negative (typically, because the chemistry is "fast", and one or more reactions are near-equilibrium), the step size is repeatedly halved until either the species mole fraction becomes positive or the step size becomes less than

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* Applying the same criteria to the momentum and energy equations usually results in larger values of $(\Delta x)_{max}$.

some minimum step size.* In the latter case, the program terminates. After the species mole fraction becomes positive, the next value of Δx is again computed from $\frac{1}{3}(\Delta x)_{max}$. Thus the step size is never determined from the value of Δx needed to satisfy stability for the previous step. This is a somewhat unique approach to specifying Δx for the solution to finite difference equations, and can save substantial computer time. It was adopted because, typical rocket plume calculations show that, when using the mixed implicit/explicit difference scheme, the chemistry only influences stable step sizes in a small region of the flow. Once the program integrates through this region step sizes of $\frac{1}{3}(\Delta x)_{max}$ usually suffice.

B. Edge of Mixing Layer

An additional radial mesh point (at free stream conditions) is added whenever the "next-to-the-last" radial point value of temperature or velocity, differs from the corresponding free stream value by more than a specified percentage of the free stream value. One percent has been selected for velocity and five percent for temperature.

C. Halving the Mesh

The number of grid points cannot be allowed to expand without bounds because of the limited storage capacity of the computer. Therefore, the number of points is halved either when the mesh increases to twice its original size (Card 2, Cols. 1-5) or the number of points exceeds 26. The computer prints all output at the station at which halving occurs.

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*The minimum step size is an input number (Card 5, Cols 1-10).

IV. CHEMICAL REACTION RATE EQUATIONS

Ten possible reaction types are included in the program:

Reaction Type

(1)	$A + B \rightleftarrows C + D$
(2)	$A + B + M \rightleftarrows C + M$
(3)	$A + B \rightleftarrows C + D + E$
(4)	$A + B \rightleftarrows C$
(5)	$A + M \rightleftarrows C + D + M$
(6)	$A + B \rightarrow C + D$
(7)	$A + B + M \rightarrow C + M$
(8)	$A + B \rightarrow C + D + E$
(9)	$A + B \rightarrow C$
(10)	$A + M \rightarrow C + D + M$

Reaction types (6)-(10) correspond to reaction types (1)-(5), but proceed in the forward direction only. In Reactions (2), (5), (7) and (10), M is an arbitrary third body. In this program, all species are assumed to have equal third body efficiencies; thus, in evaluating $\dot{w}^{(j)}$, $F_M = (W)^{-1}$. The net rates of production for all reactions are written below, in the form, $\dot{w}^{(j)} = RP^{(j)} - RM^{(j)}$.*

(1) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^2 F_C F_D}{K_p}$$

(2) $$\dot{w}^{(j)} = \frac{k_f \rho^3 F_A F_B}{W} - \frac{k_f \rho^2 F_C}{K_p\, WRT}$$

(3) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C F_D F_E RT}{K_p}$$

(4) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B - \frac{k_f \rho^3 F_C}{K_p\, RT}$$

(5) $$\dot{w}^{(j)} = \frac{k_f \rho^2 F_A}{W} - \frac{k_f \rho^3 F_C F_D RT}{K_p\, W}$$

---

* The symbols RP and RM are used on the computer output.

(6) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B$$

(7) $$\dot{w}^{(j)} = \frac{k_f \rho^3 F_A F_B}{W}$$

(8) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B$$

(9) $$\dot{w}^{(j)} = k_f \rho^2 F_A F_B$$

(10) $$\dot{w}^{(j)} = \frac{k_f \rho^2 F_A}{W}$$

To reduce round-off and truncation errors $RP^{(j)}$ and $RM^{(j)}$ are computed separately for each reaction. All contributions to the molar rate of production of a given species are then computed and added algebraically to form $\dot{w}_i$.

The forward rate coefficient, k_f, is expressed in the form,

$$k_f = AT^{-N} \exp(B/RT) \tag{23}$$

and K_p is determined from,

$$\ln K_p = -\Delta G/RT \tag{24}$$

The rate coefficients are divided into seven types:

Rate Coefficient Type*

(1) $k_f = A$

(2) $k_f = AT^{-1}$

(3) $k_f = AT^{-2}$

(4) $k_f = AT^{-\frac{1}{2}}$

(5) $k_f = A \exp(B/RT)$

(6) $k_f = AT^{-1} \exp(B/RT)$

(7) $k_f = AT^{-\frac{3}{2}}$

*Rate coefficient data for typical rocket plume reactions may be found, e. g., in Ref. 15.

V. THERMODYNAMIC DATA

The thermodynamic properties (specific heat, Gibbs free energy and enthalpy) for each species are taken directly from the JANNAF Thermochemical Tables,[16] and input to the program as c_{p_i}, $-\left(\frac{g_i - h_{298_i}}{T}\right)$ and $(h_i - h_{298})$ in tabular form as a function of temperature (Card 11). Linear interpolation is used to define thermodynamic properties at the local temperature.

VI. TRANSPORT PROPERTIES

A. Turbulent Eddy Viscosity Models

The following eddy viscosity models[17-20] are incorporated into the program:

Model 1 (Ferri)[17]

Initial region,*

$$\mu = \rho \epsilon = \alpha 0.00137 \, x \, | \rho_o u_o - \rho_e u_e | \qquad (25a)$$

Developed region,

$$\mu = \rho \epsilon = \alpha K \, b_{\frac{1}{2}} \, | \rho_o u_o - \rho_e u_e | \qquad (25b)$$

where $b_{\frac{1}{2}}$ is the value of r where $\rho u = (\rho_o u_o + \rho_e u_e)/2$ and K is the eddy viscosity coefficient, usually taken to be 0.025.†

---

*Defined as region upstream of axial position where $(u_o - u_e)/(u_j - u_e) = 0.95$.

†Most of the models contain a numerical coefficient K which must be determined empirically. The value K = 0.025, taken from Schlicting,[18] has been incorporated directly into the program. This can be changed by the program input data via an appropriate value for the additional constant, α, Eqs. (25-31) (Card 4, Cols. 61-70).

Model 2 (Ting/Libby)[19]

$$\mu = \rho \epsilon = \alpha K \bar{r}_{\frac{1}{2}} \left| u_o - u_e \right| \rho \left(\frac{\rho_o}{\rho}\right)^2 \left(\frac{\eta}{r}\right)^2 \tag{26}$$

where

$$\eta^2 = 2 \int_0^r (\rho_o/\rho)\, r'\, dr' \tag{27}$$

and $\bar{r}_{\frac{1}{2}}$ is the value of η where $u = (u_o + u_e)/2$

Model 3

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 \times \rho_o \left| u_o - u_e \right| \tag{28a}$$

Developed region,

$$\mu = \alpha K r_{\frac{1}{2}} \rho_o \left| u_o - u_e \right| \tag{28b}$$

where $r_{\frac{1}{2}}$ is the value of r where $u = (u_o - u_e)/2$

Model 4

Initial region,

$$\mu = \rho \epsilon = \alpha 0.00137 \times \rho_e \left| u_o - u_e \right| \tag{29a}$$

Developed region,

$$\mu = \rho \epsilon = \alpha K r_{\frac{1}{2}} \rho \epsilon \left| u_o - u_e \right| \tag{29b}$$

Model 5* (Ting/Libby)[19]

Initial region,

$$\mu = \rho\epsilon = \alpha 0.00137 \times |u_j - u_e| \rho\left(\frac{\rho_j}{\rho}\right)^2 \qquad (30)$$

Developed region,

$$\mu = \rho\epsilon = \alpha K \bar{r}_{\frac{1}{2}} |u_o - u_e| \rho\left(\frac{\rho_o}{\rho}\right)^2 \left(\frac{r}{r_1}\right)^2 \qquad (26)$$

Model 6 (Donaldson/Gray)[20]

Initial region,

$$\mu = \rho\epsilon = \alpha \bar{K} (r_{\frac{1}{2}} - r_i) \rho |u_o - u_e|/2 \qquad (31a)$$

$$\text{For } M_{\frac{1}{2}} \leq 1.2 \quad \bar{K} = 0.0468 + M_{\frac{1}{2}} \left[-0.0460 M_{\frac{1}{2}} + 0.0256 M_{\frac{1}{2}}^2 \right]$$

$$M_{\frac{1}{2}} > 1.2 \quad \bar{K} = 0.0248 \qquad (32)$$

where $M_{\frac{1}{2}}$ is the value of the Mach number where $u = (u_o + u_e)/2$ (i.e., the half radius). The speed of sound at the half radius, $a_{\frac{1}{2}}$, is expressed by,

$$a_{\frac{1}{2}} = \left[\frac{c_p}{c_p - (R/W_{\frac{1}{2}})} \frac{RT_{\frac{1}{2}}}{W_{\frac{1}{2}}} \right]^{\frac{1}{2}} \qquad (33)$$

where $W_{\frac{1}{2}}$ and $T_{\frac{1}{2}}$ are evaluated at the half radius. In Eq. (31a), r_i is the inner mixing zone radius and is defined as the value of r where $(u - u_e)/(u_j - u_e) = 0.95$.

Developed region,

$$\mu = \rho\epsilon = \alpha \bar{K} r_{\frac{1}{2}} \rho |u_o - u_e|/2 \qquad (31b)$$

---

*In the program, the specification of Model 5 means that Eq. (30) will be used in the initial region and Model 2 (Eq. 26) will be used in the developed region. This is important for re-starting a problem in the developed region for which Model 5 was selected to run from x = 0. In this case, Model 2 must be specified on Card 2, Cols. 11-15.

B. Laminar Flow

Sutherland's Law[21] is used to describe the viscosity as a function of temperature.

$$\mu = 9.8 \times 10^{-7} T^{3/2} / (T + 111) \qquad lb_m/ft\text{-}sec \qquad (34)$$

VII. PLUME ELECTRICAL PROPERTIES

Electron density, electron-neutral collision frequency, unit radar attenuation and electrical conductivity are computed at all radial points for each axial print-out station.

A. Electron Density

$$n_e = 0.733\,(10^{22})\, X_{e^-}\, p\, T^{-1} \qquad m^{-1} \qquad (35)$$

where p is in atm and T in degrees K.

B. Collision Frequency

$$\nu_e = 4.57\,(10^{27})\, p\, T^{-\frac{1}{2}} \sum_i X_i\, Q_{e_i} \quad sec^{-1} \qquad (36)$$

where p is in atm, T in degrees K and Q_{e_i} in cm^2. The electron-neutral collision cross sections[22] used in the calculations and given in the following table are those which characterize typical solid propellant exhaust plumes. If other species contribute to the value of ν_e, the program must be modified.

Species	Q_{ei}, cm^2
CO	$2.03\ (10^{-23})\nu_e^{\dagger} + 2.46\ (10^{-16})$
CO_2	$4.7\ (10^{-8})\nu_e^{-1}$
H_2O	$5.9\ \nu_e^{-2}$
HCl	$1.85\ \nu_e^{-2}$
N_2	$3.29\ (10^{-23})\nu_e$
H_2	$1.45\ (10^{-23})\nu_e + 8.7\ (10^{-16})$

$^{\dagger}\ \nu_e = 6.21\ (10^5)\ T^{\frac{1}{2}}$ cm/sec

C. Transverse Radar Attenuation

$$a' = 1.17\ \frac{n_e/\nu_e}{[1 + (\omega/\nu_e)^2]} \qquad \text{db/in} \tag{37}$$

where n_e is in ml^{-1}, ν_e in sec^{-1} and ω is rad/sec.* The program then computes transverse (normal to the axis) radar attenuation along a "line-of-site" (i.e. radar beam "spot size" much smaller than the electrical plume diameter) from,

$$A = 2\int_0^{\infty} a'\ dr \qquad \text{db} \tag{38}$$

where r is in inches.

D. Electrical Conductivity

$$\sigma = 2.54(10^4)\ \frac{e^2\, n_e}{\nu_e\, m_e} \quad \text{mho/in} \tag{39}$$

where e is 1.6×10^{-19} coulomb and m_e is 9.1×10^{-31} kg.

*Attenuation calculations can be made for a maximum of six signal frequencies.

VIII. PROGRAM OPERATION

A. Machine

The program, as listed in Appendix A, must be run on a CDC computer since a library routine named SECOND (called in subroutine TICK) is used to sense elapsed time from the start of execution. This routine enables the continuing solution cards to be punched when the execution time exceeds the time input on Card 2, Cols. 36-40--if punch options 2 or 3 are selected (Card 2, Cols. 31-35). The program may be run on a different machine by removing the subroutine and replacing it with the dummy routine shown below:

```
SUBROUTINE TICK (JJJ)
JJJ = 0
RETURN
END
```

When this is done the maximum execution time input on Card 2, Cols. 36-40 will not trigger the punch option.

Input and output are on the standard tape units (i.e. 5 for READ, 6 for WRITE and 7 for PUNCH).

B. Sense Switch Control

1. Sense Switch 1 - When Sense Switch 1 is on, the current values of x, T_o, and $n_{e,o}$ are printed on-line.

2. Sense Switch 3 - When Sense Switch 3 is on, the case is terminated and all output is printed at the current axial station.

C. Program Optimization

It is recommended that the program be compiled using the highest level of optimization. On the CDC 6600 this corresponds to the FAST OBJECT CODE MODE.

IX. PROGRAM INPUT DATA

The input data cards are explained below. A listing of the computer program, a sample input data sheet and a sample output are given in Appendices A, B and C, respectively.

Card No.	Columns	Description	Format
1	1-72	Run identification	12A6
2	1-5	Initial number of grid points* in ψ coordinate (26 maximum)	I5
	6-10	Number of species (21 maximum)	I5
	11-15	Viscosity option key If -1: Laminar (Eq. 34) 0: μ = constant 1: Model 1 (Eq. 25) 2: Model 2 (Eq. 26) 3: Model 3 (Eq. 28) 4: Model 4 (Eq. 29) 5: Model 5 (Eqs. 26 and 30) 6: Model 6 (Eq. 31)	I5
	16-20	Number of reactions (40 maximum)	I5
	21-25	$\dot{w}_i$ output option If 0: $\dot{w}_i$ for each species is not output 1: $\dot{w}_i$ for each species is output at all radial points whose temperature is greater than the kinetics cut-off temperature (Card 6, Cols. 61-70)	I5

*Recommended number, 13

Card No.	Columns	Description	Format
2	26-30	RP, RM output option If 0: RP, RM for each reaction is not output 1: RP, RM for each reaction is output at all radial points whose temperature is greater than the kinetics cut-off temperature (Card 6, Cols. 61-70)	I5
	31-35	Card punch option If 0: No cards punched 1: Cards with radial distributions of electron density and collision frequency at all printout stations are punched 2: Cards for continuing a given solution are punched 3: Both the above sets of cards are punched	I5
	36-40	Maximum computer execution time (min) (If card punch option 1, 2 or 3 is selected, cards will be punched after this amount of computer time)*	I5
	41-45	Pressure option If 0: Pressure is a constant 1: Pressure is a function of axial distance	I5
3	1-10 . . . 51-60	Signal frequencies (MHz) - 6 maximum - for which transverse attenuation calculations will be made (see Section VII). Leave blank if no attenuation calculations desired	E10.3

*In practice if this option is selected, the calculations will terminate at an execution time 30 seconds less than this value.

Card No.	Columns	Description	Format
4	1-10	Initial value of x (ft)	E10.3
	11-20	Final value of x (ft)	E10.3
	21-30	Print increment (ft)	E10.3
	31-40	Lewis number	E10.3
	41-50	Prandtl number	E10.3
	51-60	Nozzle (jet) radius (ft)	E10.3
	61-70	α, factor used to vary eddy viscosity* (see Section VI)	E10.3
5	1-10	Δx_{min}, Minimum integration step size (ft)†	E10.3
	11-20	FDL, diffusion step size factor‡	E10.3
	21-30	c_0 (atm)	E10.3
	31-40	c_1 (atm/ft)	E10.3
	41-50	c_2 (atm/ft^2) (Pressure Coefficients (see Section II))	E10.3
	51-60	c_3 (atm/ft^3)	E10.3
6	1-10	Pressure at initial value of x(atm)	E10.3
	11-20	Temperature at jet centerline (K)	E10.3
	21-30	Temperature at edge of jet (K) (free stream value)	E10.3

*Set $\alpha = 1.0$ if no changes to eddy viscosity coefficient are desired.

†Recommended value, 1×10^{-10} ft.

‡Set FDL = 1.0 if maximum integration step size criterion discussed in Section III is to be used.

Card No.	Column	Description	Format
6	31-40	Velocity at jet centerline (ft/sec)	E10.3
	41-50	Velocity at edge of jet (ft/sec) (free stream value)	E10.3
	51-60	$\Delta\Psi$, $(\frac{lbm}{32.2}\ sec^{-1})^{\frac{1}{2}}$	E10.3
		If $\Delta\Psi = 0$ (or blank) the program computes $\Delta\Psi$ assuming velocity, temperature and species mole fractions are constant at initial station	
		If $\Delta\Psi$ is specified, cards 7.1 to 9.13 are read next. If $\Delta\Psi$ is not specified, card 10.1 is the next card read with cards 7.1 through 9.13 being omitted	
	61-70	Kinetics cut-off temperature (kinetics are frozen at temperatures below this value*)	E10.3
NOTE: For the purpose of illustration it is assumed that there are 13 initial grid points in the Ψ coordinate.			
7.1	1-10	T(1), Temperature (K) at jet centerline, r = 0	E10.3
	61-70	T(7)	
7.2	1-10	T(8)	E10.3
	51-60	T(13), Temperature (K) in free stream	
8.1	1-10	u(1), Velocity (ft/sec) at jet centerline, r = 0	E10.3
	61-70	u(7)	
8.2	1-10	u(8)	E10.3
	51-60	u(13)	

*If blank or zero, 400 K is used.

Card No.	Column	Description	Format
NOTE: For the purpose of illustration it is assumed that there are 8 species			
9.1.1	1-10	Mole fraction of 1st species at jet centerline, r = 0	E10.3
	. . .		
	61-70	Mole fraction of 7th species at jet centerline, r = 0	E10.3
9.1.2	1-10	Mole fraction of 8th species at jet centerline, r = 0	E10.3
9.2.1	1-10	Mole fraction of 1st species at next grid point	E10.3
	. . .		
	61-70	Mole fraction of 7th species at next grid point	
9.2.2	1-10	Mole fraction of 8th species of next grid point	E10.3
9.13.1	1-10	Mole fraction of 1st species at 13 grid point (free stream)	E10.3
	. . .		
	61-70	Mole fraction of 7th species at 13th grid point (free stream)	
9.13.2	1-10	Mole fraction of 8th species at 13th grid point (free stream)	E10.3
NOTE: Card Type 10 is not required if Card Types 7, 8 and 9 are input.			
10.1.1	1-10	Mole fraction of 1st species at jet centerline, r = 0	E10.3
	. . .		
	61-70	Mole fraction of 7th species at jet centerline, r = 0	
10.1.2	1-10	Mole fraction of 8th species at jet centerline, r = 0	

Card No.	Column	Description	Format
10 2.1	1-10	Mole fraction of 1st species in free stream	E10.3
	61-70	Mole fraction of 7th species in free stream	
10.2.2	1-10	Mole fraction of 8th species in free stream	

NOTE: The following cards contain the thermodynamic data.* The first card contains the species name, molecular weight and heat of formation. The second and remaining cards contain the temperature and corresponding specific heat, free energy and enthalpy for that species. Two temperatures and corresponding thermodynamic data are placed on each card. The input table can contain up to a maximum of 30 temperature points. The data are input exactly as presented in the JANNAF tables.[16]

Card No.	Column	Description	Format
11.1.1	1- 6	Name of first species	A6
	7-16	Molecular weight	E10.3
	17-26	Heat of formation, h_{298_i} (kcal/mole)	E10.3
11.1.2	1-10	First temperature point (K)	E10.3
	11-20	c_{p_i} (cal/mole-K)	E10.3
	21-30	$-\left(\frac{g_i - h_{298_i}}{T}\right)$ (cal/mole K)	E10.3
	31-40	$h_i - h_{298_i}$ (kcal/mole)	E10.3
	41-50	Second temperature point (K)	E10.3
	51-60	c_{p_i} (cal/mole-K)	E10.3
	61-70	$-\left(\frac{g_i - h_{298_i}}{T}\right)$ (cal/mole-K)	E10.3

*The order of the species must be identical to the order on Card Types 9 or 10.

Card No.	Column	Description	Format
11.1.2	71-80	$h_i - h_{298_i}$ (kcal/mole)	E10.3
11.1.3	⋮	Third temperature point	
11.2.1	⋮	Name of second species	

NOTE: The chemical reaction mechanism for a particular probem is input on the last set of cards, one card for each reaction. (See Section IV.) No particular order is required.

12.1	1-6	Species A	A6
	7	+ sign	
	8-13	Species B (or M)	A6
	14	+ sign	
	15-20	Blank or M	6x
	21	= sign	
	22-27	Species C	A6
	28	+ sign (if needed)	
	29-34	Species D (or M)	A6
	35	+ sign (if needed)	
	36-41	Species E (or M)	A6
	42-48	Blank	
12.1	49-50	Reaction type, 1 to 10 (see Section IV)	I2
	51	Rate coefficient type, 1 to 7 (see Section IV)	I1
	52-59	A, Pre-exponential factor cm-molecule-sec units	E8.2
	60-63	N, Temperature exponent	F4.1
	64-72	B, Activation energy cal/mole	F9.1
12.2	⋮	Next Reaction	

X. PROGRAM OUTPUT

A. Description

Sample output sheets for the input data given in Appendix B are shown in Appendix C. The first page contains the key program input parameters, initial distributions of velocity, temperature and species mole fractions and the chemical reaction mechanism and rate coefficients. The succeeding pages contain printouts at axial stations corresponding to the print increment (Card 4, Cols. 21-30). Following the listing of electrical properties (last page of output), the integration step size and corresponding axial position are given for each integration step up to the next print station.

B. Units

A mixed system of units appears on the program output for ease in making additional calculations and for program check-out.

COLLISION FREQUENCY	electron-neutral collision frequency, sec^{-1}.
DELTA X	integration step size, ft
DENSITY	g/cm^3
ELECTRICAL CONDUCTIVITY	mho/in
ELECTRON DENSITY	ml^{-1}
ENTHALPY	mixture static enthalpy, cal/g
HALF RADIUS/R	nondimensional radial distance to point where $u = (u_o + u_e)/2$, ft (viscosity option 6 only)
INNER MIXING ZONE RADIUS/R	nondimensional radial distance to point where $(u-u_e)/(u_j - u_e) = 0.95$, (viscosity option 6 only)
MACH NO.	Mach number
MACH NUMBER AT HALF RADIUS	Mach number at point where $u = (u_o + u_e)/2$ (viscosity option 6 only)
MINIMUM STEP SIZE	$(\Delta x)_{min}$, ft

MIXING RATE COEFFICIENT	defined by Eq. (31a) or Eq. (31b) (viscosity option 6 only)
MOLE FRACTIONS	species mole fractions
NET RATE OF PRODUCTION (W-DOT/RHO*U)	$\dot{w}_i/\rho u$, mole/g-ft
PRESS	pressure, atm
PSI	stream function, $\left[\frac{\text{lbm}}{32.2}\ \text{sec}^{-1}\right]^{\frac{1}{2}}$
PT	radial grid point number
R	nozzle radius
REACTION J	refers to reactions listed on first page of output
RM	negative molar rate of production for jth reaction (see Section IV), mole/ml-sec
RP	positive molar rate of production for jth reaction (see Section IV), mole/ml-sec
SIGN. FREQ.	signal frequency for attenuation calculations, mHz
TEMPERATURE	K
TRANSVERSE ATTENUATION	db
UNIT ATTENUATION	db/in
VELOCITY	axial velocity, ft/sec
VISCOSITY	μ, lbm/ft-sec
X	axial distance, ft
X/R	nondimensional axial distance
Y/R	nondimensional radial distance from axis

C. Card Output

1. Continuing Solution - Due to the large amount of input data required to continue a solution (after being terminated at a given value of x) the program will punch all input except the thermodynamic data and chemical reaction mechanism if this option is selected (Card 2, Cols. 31-35). However, a new final value of x (Card 4, Cols. 11-20) must be input manually if the problem was initially terminated by reaching the old maximum distance. Cards will also be produced if maximum time (Card 2, Cols. 36-40) is exceeded, by using the proper option.

2, Electron Density and Collision Frequency - The complete radial distribution of electron density and collision frequency at all printout stations will be punched if this option is selected (Card 2, Cols. 31-35).

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APPENDIX A

A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

Fortran Listing

```
      PROGRAM MAIN (INPUT,OUTPUT,PUNCH,TAPE5=INPUT,TAPE6=OUTPUT,          MAIN      2
     1    TAPE7=PUNCH)                                                    MAIN      3
C*************************************************************          MAIN      4
C***********                                                  **          MAIN      5
C***********          A FAST COMPUTER PROGRAM                 **          MAIN      6
C***********   FOR NONEQUILIBRIUM REENTRY PLUME PREDICTIONS    **          MAIN      7
C***********          AEROCHEM RESEARCH LABORATORIES          **          MAIN      8
C***********             PRINCETON, N. J.                     **          MAIN      9
C***********                                                  **          MAIN     10
C*************************************************************          MAIN     11
C                                                                         MAIN     12
C                                                                         MAIN     13
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),  MAIN     14
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),  MAIN     15
     2          WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),   MAIN     16
     3RU(30),U(30),TITLE(12),XLE(18),XMU(30)          ,G(30),WTMIX(30),   MAIN     17
     4RC(40,3),IRRR(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),  MAIN     18
     5          IRR(40),FREQ(30),SAVEA(25,30),          PC(4),ZID(5),    MAIN     19
     6          ECC(30),HOUT(30),YOUT(30),PHOOUT(30),XMUOUT(30),XLT(30),  MAIN     20
     7T4(30),TFDG(30),IRT(40),RP(40,30),RM(40,30)                         MAIN     21
     8 ,CM(25,25,26), DX(25,26) ,CMI(25,25),DXI(25)                       MAIN     22
      DIMENSION XAME(6), ISAVE(6), FREQA(6), ALOG(50,6)                   MAIN     23
      DIMENSION TTB(30)    ,CPTB(25,30),HTB(25,30),UTB(25,30),HF(25)      MAIN     24
      COMMON  A       , RHO     , Y       , T       , PSI     , RT        MAIN     25
      COMMON  SUM     , AR      , HSTAT   , H       , ALPHA   , RALPHA    MAIN     26
      COMMON  CP      , SIGMA             , WTMOLE  , CPBAR   , C         MAIN     27
      COMMON  AID     , ETA     , RATIO   , RU      , U       , TITLE     MAIN     28
      COMMON  XLE     , XMU     ,         , G       , WTMIX   , WDOT      MAIN     29
      COMMON  SAVEU   , SAVET   , WM      , WP      , RC                    MAIN     30
      COMMON            SAVEA   ,         , PC      , X       , XMAX      MAIN     31
      COMMON  PRNT    , DXMIN   , DX      , EPL     , OPTPST  , II        MAIN     32
      COMMON  XR2     , P       , ZID     , FREQ    , ECC     , DPDX      MAIN     33
      COMMON  YOUT    , HOUT    , PHOOUT  , IRRR    , IRR     , IFIRIR    MAIN     34
      COMMON  IPAGE   , NPSI    , MY      , NS      , NR      , IFDGL     MAIN     35
      COMMON  ITURB   , IPRESS  , NPSI    , IICST   , IICR    , IFCC      MAIN     36
      COMMON  IRT     , XMUOUT  , XLT     , T4      , TFDG    , IDUT      MAIN     37
      COMMON  IOUTI   , IOUT2   ,RP       , RM      , ISAVE   , IPUNCH    MAIN     38
      COMMON IKINET,NFREQA,ALOG,FREQA,00100,00200,00300,00400             MAIN     39
C**** SETTING XAME FOR THOSE SPECIES INVOLVED IN COLLISION FREQ. CALC.    MAIN     40
      DATA XAME(1)/6HCO    /                                              MAIN     41
      DATA XAME(2)/6HCO2   /                                              MAIN     42
      DATA XAME(3)/6HH2O   /                                              MAIN     43
      DATA XAME(4)/6HH2    /                                              MAIN     44
      DATA XAME(5)/6HN2    /                                              MAIN     45
      DATA XAME(6)/6HOHCL  /                                              MAIN     46
      AV=6.025E23                                                         MAIN     47
    4 IFINIS=0                                                            MAIN     48
      DO 9999 I=1,8596                                                    MAIN     49
 9999 A(I)=0.0                                                            MAIN     50
      DO 300 I = 1,6                                                      MAIN     51
  300 ISAVE(I) = 0                                                        MAIN     52
      P=42.06                                                             MAIN     53
      READ  (5,333)(TITLE(I),I=1,12)                                      MAIN     54
C     NS= NO. OF SPECIES                                                  MAIN     55
C     NR= NO. OF REACTIONS                                                MAIN     56
```

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PROGRAM     MAIN                                  CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  13.44.49.      PAGE
                READ(5,100) MPSI,NS,ITURB,IR,IOUT1,IOUT2,IPUNCH,ITIME,IPRESS,NT      MAIN       97
                READ (5,111)  (FREQA(I), I=1,6)                                      MAIN       98
                DO 113 I=1,6                                                         MAIN       99
                IF (FREQA(I)) 113, 114, 113                                          MAIN      100
 60           113 CONTINUE                                                          MAIN      101
                I=7                                                                  MAIN      102
              114 NFREQA = I-1                                                       MAIN      103
                NPSI=MPSI-1                                                          MAIN      104
                READ  (5,1000)X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2                    MAIN      105
 65             DX=0.1*RJ                                                          MAIN      106
C               INPUT MINIMUM STEPSIZE LIMIT (DXMIN)                               MAIN      107
                READ(5,1000) DXMIN,FOL,      PC(1),PC(2),PC(3),PC(4)               MAIN      108
                READ  (5,1000)P,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET            MAIN      109
                IF(TKINET.EQ.0.0) TKINET = 400.0                                   MAIN      110
 70           C**** THE VALUE OF 30 SECONDS IS TO ALLOW FOR COMPILE TIME            MAIN      111
                TLIMIT = 60*ITIME-30                                               MAIN      112
                IDIFFT = 0                                                         MAIN      113
                CALL TICK(ISECST)                                                  MAIN      114
                IF((ISECST+60*ITIME).GT.86400) IDIFFT = 86400-ISECST               MAIN      115
 75             UNIT = U(1)                                                        MAIN      116
                IQ77 = 2                                                           MAIN      117
                USURO1 = 0.0                                                       MAIN      118
C               TURBULENCE MODELS                                                  MAIN      119
                IF (ITURB - 3) 8600,9010,9010                                      MAIN      120
 80           8600 IF (ITURB - 1) 9011,9010,9011                                   MAIN      121
              9010 USURO1 = 0.95*   (U(1)-U(MPSI)) + U(MPSI)                       MAIN      122
              9011 CONTINUE                                                        MAIN      123
                IF(DELPSI) 3011,3012,3011                                          MAIN      124
              3012 READ  (5,1000)(ALPHA(J,1),J=1,NS)                               MAIN      125
 85             READ  (5,1000)(ALPHA(J,MPSI),J=1,NS)                               MAIN      126
                MMOD=MPSI-2                                                        MAIN      127
                DO 4001 I=1,MMOD                                                   MAIN      128
                T(I)=T(I)                                                          MAIN      129
                U(I)=U(I)                                                          MAIN      130
 90             DO 4001 J=1,NS                                                     MAIN      131
              4001 ALPHA(J,I)=ALPHA(J,1)                                           MAIN      132
                DO 4002 J=1,NS                                                     MAIN      133
              4002 ALPHA(J,NPSI)=ALPHA(J,MPSI)                                     MAIN      134
                GO TO 3015                                                         MAIN      135
 95           3011 READ  (5,1000)(T(I),I=1,MPSI)                                   MAIN      136
                READ  (5,1000)(U(I),I=1,MPSI)                                      MAIN      137
                DO 7 I=1,MPSI                                                      MAIN      138
              7 READ  (5,1000)(ALPHA(J,I),J=1,NS)                                  MAIN      139
C               NEW THERMO DATA DATA INPUT IN JANNAF TABLE FORM                    MAIN      140
100          3015 DO 1991 I=1,NS                                                   MAIN      141
                READ(5,222) AID(I),WTMOLE(I),HF(I)                                 MAIN      142
                DO 10 IT=1, N1,2                                                   MAIN      143
                READ(5,102) TTB(IT),  CPTB(I,IT),GTB(I,IT),HTB(I,IT)              MAIN      144
               1   ,TTB(IT+1)  ,CPTB(I,IT+1), GTB(I,IT+1),HTB(I,IT+1)             MAIN      145
105             GTB(I,IT)= -GTB(I,IT)*TTB(IT)  +HF(I) *1000.                      MAIN      146
                GTB(I,IT+1)= -GTB(I,IT+1)*TTB(IT+1)  +HF(I)*1000.                  MAIN      147
                HTB(I,IT)=(HTB(I,IT)+HF(I))*1000.                                  MAIN      148
                HTB(I,IT+1)=(HTB(I,IT+1)+ HF(I))*1000.                             MAIN      149
             10 CONTINUE                                                           MAIN      150
110             IF(WTMOLE(I)-1.0) 1972,1991,1991                                   MAIN      151
```

```
      1972 IECC=1                                                          MAIN      112
      1991 CONTINUE                                                        MAIN      113
           DO 301 J = 1,6                                                  MAIN      114
           DO 301 I = 1,NS                                                 MAIN      115
  115      IF(AID(I).EQ.XAME(J)) ISAVE(J) = I                              MAIN      116
       301 CONTINUE                                                        MAIN      117
           DO 1992 I=1,NR                                                  MAIN      118
           READ  (5,444)(ZID(J),J=1,5),IRR(I),IRT(I),(RC(I,K),K=1,3)       MAIN      119
           DO 1993 J=1,5                                                   MAIN      120
  120      IRR(I,J)=0                                                      MAIN      121
           DO 1993 L=1,NS                                                  MAIN      122
           IF(ZID(J)-AID(L)) 1993,1994,1993                                MAIN      123
      1994 IRR(I,J)=L                                                      MAIN      124
      1993 CONTINUE                                                        MAIN      125
  125 1992 CONTINUE                                                        MAIN      126
           DO 912 I=1,MPSI                                                 MAIN      127
           WTVR=0.0                                                        MAIN      128
           DO 632 J=1,NS                                                   MAIN      129
       632 WTVR=WTVR+ALPHA(J,I)*WTHOLE(J)                                  MAIN      130
  130      DO 633 J=1,NS                                                   MAIN      131
       633 ALPHA(J,I)=ALPHA(J,I)/WTVR                                      MAIN      132
       912 CONTINUE                                                        MAIN      133
           IF(DELPSI) 903,3041,903                                         MAIN      134
      3041 DUM=0.0                                                         MAIN      135
  135      DO 5001 J=1,NS                                                  MAIN      136
      5001 DUM=DUM+ALPHA(J,1)                                              MAIN      137
           XMD=MMOD-1                                                      MAIN      138
           DELPSI=SQRT(P*U(1)/42.205/T(1)/DUM)*RJ/XMD                      MAIN      139
       903 DO 20 I=1,29                                                    MAIN      140
  140      XI=I-1                                                          MAIN      141
           PSI(I)=XI*DELPSI                                                MAIN      142
           XLE(I)=XLE(1)                                                   MAIN      143
        20 SIGMA(I)=SIGMA(1)                                               MAIN      144
           DO 90 I=MPSI,29                                                 MAIN      145
  145      RT(I)=T(MPSI)                                                   MAIN      146
           T(I)=T(MPSI)                                                    MAIN      147
           DO 80 J=1,NS                                                    MAIN      148
           RALPHA(J,I)=ALPHA(J,MPSI)                                       MAIN      149
        80 ALPHA(J,I)=ALPHA(J,MPSI)                                        MAIN      150
  150      RU(I)=U(MPSI)                                                   MAIN      151
        90 U(I)=U(MPSI)                                                    MAIN      152
           CALL  INOUT                                                     MAIN      153
           PPUNCH = P                                                      MAIN      154
           P=2117.0*P                                                      MAIN      155
  155      DPDX=0.0                                                        MAIN      156
C           PRESSURE OPTION.  IF IPRESS= 0,  PRESSURE                      MAIN      157
C           IS CONSTANT AND = TO P. IF IPRESS = 1, COEFFICIENTS CALLED     MAIN      158
C           PC(1),PC(2),PC(3),PC(4) ARE INPUT.                             MAIN      159
C           EQUATION USED IS P = PC(1) + PC(2)*X + PC(3)*X*X + PC(4)*X*X*X MAIN      160
  160      2 IF(IPRESS) 821,822,821                                        MAIN      161
       821 P=(PC(1)+X*(PC(2)+X*(PC(3)+X*PC(4))))*2117.0                    MAIN      162
           DPDX=(PC(2)+X*(2.0*PC(3)+X*3.0*PC(4)))*2117.0                   MAIN      163
           PPUNCH = P/2117.0                                               MAIN      164
       822 DO 31 I=1,MPSI                                                  MAIN      165
  165      WTMIX(I)=0.0                                                    MAIN      166
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 PROGRAM    MAIN                    (DC 6600 FTN V5.0-P312 OPT=2   08/07/73  12.16.49.     PAGE    8

                DO 30 J=1,NS                                                    MAIN     167
             30 WTMIX(I)=WTMIX(I)+ALPHA(J,I)                                    MAIN     168
                RHO(I)=P/89517.501/T(I)/WTMIX(I)                                MAIN     169
             31 RHOOUT(I)=RHO(I)/1.94                                           MAIN     170
    170         DO 805 I=1,MPSI                                                 MAIN     171
           C    FREE STREAM VELOCITY WILL BE SET TO 1.0 FPS IF ZERO IS ENTERED  MAIN     172
                U(I) = AMAX1(1.0,U(I))                                          MAIN     173
                TFOG(I)=AMAX1((T(I)-100.00)                                     MAIN     174
                T4(I)=TFOG(I)**4                                                MAIN     175
    175         XLT(I)=ALOG(TFOG(I))                                            MAIN     176
                CPBAR(I)=0.0                                                    MAIN     177
                HSTAT(I)=0.0                                                    MAIN     178
                TX=T(I)                                                         MAIN     179
                CALL TKEY(TX  ,TTB,ITKEY,SDT,HDT,NT)                            MAIN     180
    180         IF (ITKEY.EQ.0) GO TO 9                                         MAIN     181
                DO 805 J=1,NS                                                   MAIN     182
                CP(J,I)=0.0                                                     MAIN     183
                H(J,I)=0.0                                                      MAIN     184
                CALL LIPLN(ITKEY,J,CPTB,SDT,HDT,AX)                             MAIN     185
    185         CP(J,I)=AX*45055.31                                             MAIN     186
                CALL LIPLN(ITKEY,J, HTB,SDT,HDT,AX)                             MAIN     187
                H(J,I)=AX*45055.31                                              MAIN     188
                HSTAT(I)=HSTAT(I)+H(J,I)*ALPHA(J,I)                             MAIN     189
            805 CPBAR(I)=CPBAR(I)+CP(J,I)*ALPHA(J,I)                            MAIN     190
    190         ETA(1)=0.0                                                      MAIN     191
                Y(1)=0.0                                                        MAIN     192
                ETA(2)=DELPSI/SQRT(RHO(1)*U(2))                                 MAIN     193
                Y(2)=DELPSI/SQRT(RHO(2)*U(2))                                   MAIN     194
                DO 25 I=3,MPSI                                                  MAIN     195
    195         ETA(I)=SQRT(ETA(I-2)**2+DELPSI*(PSI(I)/U(I)+4.0*PSI(I-1),U(I-1)+PS MAIN     196
               1(I-2)/U(I-2))/1.5/RHO(1))                                       MAIN     197
                TEMP = (Y(I-2)**2+DELPSI*(PSI(I)/RHO(I)/U(I)+4.0*PSI(I-1; RHO(I-1) MAIN     198
               1    /U(I-1)+PSI(I-2)/RHO(I-2)/U(I-2))/1.5)                      MAIN     199
                IF(TEMP.LT.0.0) CALL OUTPUT                                     MAIN     200
    200      25 Y(I) = SQRT(TEMP)                                               MAIN     201
           C**** HAS MIXING REGION INTERSECTED X AXIS YET, YES IF 0 OR =        MAIN     202
                IF (ITURB-6) 8010,8011,8010                                     MAIN     203
            8010 IF (U(1) - USUB01) 9000,9000,900)                              MAIN     204
           C    MODEL 6 COMMON CALCULATIONS                                     MAIN     205
    205     8011 Q01 = (U(1)+U(MPSI))/2.0                                       MAIN     206
                DO 8012 I=2,MPSI                                                MAIN     207
                IF ((Q01-U(I))*(Q01-U(I-1))) 8013,8013,8012                     MAIN     208
            8012 CONTINUE                                                       MAIN     209
            8013 Q02 = (Q01-U(I-1))/(U(I)-U(I-1))                               MAIN     210
    210         Q0100 = Y(I-1)+(Y(I)-Y(I-1))*Q02                                MAIN     211
                Q030 = T(I-1)+(T(I)-T(I-1))*Q02                                 MAIN     212
                Q03 = CPBAR(I-1)+(CPBAR(I)-CPBAR(I-1))*Q02                      MAIN     213
                Q04 = 1.0/(WTMIX(I-1)+(WTMIX(I)-WTMIX(I-1))*Q02)                MAIN     214
                Q05 = 89517.501/Q04                                             MAIN     215
    215         Q06 = Q03/(Q03-Q05)                                             MAIN     216
                Q07 = SQRT(Q06*Q05*Q030)                                        MAIN     217
                Q0300 = Q01/Q07                                                 MAIN     218
                Q0R = (ABS(U(1)-U(MPSI)))/2.0                                   MAIN     219
                IF (Q0300-1.2) 8014,8014,8015                                   MAIN     220
    220     8014 Q0400 =(.0468+Q0300*((Q0300*(-.0460))+.0256*(Q0300*Q0300)))*XK2 MAIN     221
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```
      GO TO 8016                                                        MAIN      222
 8015 QQ400 = .0248*XK2                                                 MAIN      223
 8016 IF ((U(1)-USUB01)*(U(1)-U(MPSI))) 8020,8020,8800                  MAIN      224
 8020 IF (USUB01-9000.0) 8021,8021,8900                                 MAIN      225
  225 8021 USUB01 = 10000.0                                             MAIN      226
      WRITE (6,9900) X                                                  MAIN      227
      GO TO 8900                                                        MAIN      228
C     MODEL 6 BEFORE MIXING ZONE REACHES AXIS                           MAIN      229
 8800 QQ9 = 0.95*   (U(1)-U(MPSI)) + U(MPSI)                           MAIN      230
  230 DO 8802 I = 2,MPSI                                                MAIN      231
      IF ((QQ9-U(I))*(QQ9-U(I-1))) 8804,8804,8802                       MAIN      232
 8802 CONTINUE                                                          MAIN      233
 8804 QQ200 = Y(I-1)+(Y(I)-Y(I-1))*(QQ9-U(I-1))/(U(I)-U(I-1))           MAIN      234
      QQ10 = QQ400*QQ8*(QQ100-QQ200)                                    MAIN      235
  235 DO 8810 I = 1,MPSI                                                MAIN      236
 8810 XMU(I) = QQ10*RHO(I)                                              MAIN      237
      GO TO 98                                                          MAIN      238
C     MODEL 6 AFTER MIXING ZONE REACHES AXIS                            MAIN      239
 8900 QQ11 = QQ400*QQ100*QQ9                                            MAIN      240
  240 DO 8910 I = 1,MPSI                                                MAIN      241
 8910 XMU(I) = QQ11*RHO(I)                                              MAIN      242
      QQ200 = 0.0                                                       MAIN      243
      GO TO 98                                                          MAIN      244
 9000 IQ77 = 9                                                          MAIN      245
  245 USUB01 = 0.0                                                      MAIN      246
      WRITE (6,9900)X                                                   MAIN      247
 9001 LL = ITURB + 1077                                                 MAIN      248
C      EDDY VISCOSITY  MODELS                                           MAIN      249
      GO TO (91,99,8666,78,8667,8668,9003,91,99,45,78,26,33,78),LL      MAIN      250
  250 C      MODEL 1 BEFORE MIXING ZONE REACHES AXIS                    MAIN      251
 8666 XMU(1)=0.00137*(X+1.0E-05)*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))     MAIN      252
      GO TO 37                                                          MAIN      253
C      MODEL 3 BEFORE MIXING ZONE REACHES AXIS                          MAIN      254
 8667 XMU(1)=0.00137*(X+1.0E-05)*RHO(1)*ABS(U(1)-U(MPSI))               MAIN      255
  255 GO TO 37                                                          MAIN      256
C      MODEL 4 BEFORE MIXING ZONE REACHES AXIS                          MAIN      257
 8668 XMU(1)=0.00137*(X+1.0E-05)*RHO(MPSI)*ABS(U(1)-U(MPSI))            MAIN      258
      GO TO 37                                                          MAIN      259
   91 DO 92 I=1,MPSI                                                    MAIN      260
C     MODEL 0 LAMINAR FLOW                                              MAIN      261
  260 92 XMU(I)=3.05E-8*T(I)**1.5/(T(I)+111.0)                          MAIN      262
      GO TO 98                                                          MAIN      263
   45 DUM=.5*(RHO(1)*U(1)+RHO(MPSI)*U(MPSI))                            MAIN      264
      DO 52 J=1,MPSI                                                    MAIN      265
  265 I=MPSI-J+1                                                        MAIN      266
      IF(RHO(I)*U(I)-DUM) 52,52,51                                      MAIN      267
   52 CONTINUE                                                          MAIN      268
C     MODEL 1 AFTER MIXING ZONE REACHES AXIS                            MAIN      269
   51 Z=Y(I)+(Y(I)-Y(I+1))*(RHO(I)*U(I)-DUM)/(RHO(I)*U(I)-RHO(I+1)*U(I+1  MAIN      270
  270   ))                                                              MAIN      271
      XMU(1)=XK2*Z*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))*0.025             MAIN      272
      GO TO 37                                                          MAIN      273
   99 DO 39 I=1,MPSI                                                    MAIN      274
   39 XMU(I)=XK2*0.025                                                  MAIN      275
  275 GO TO 98                                                          MAIN      276
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      PROGRAM    MAIN                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/78  12.54.49.    PAGE     6

                   78 RD=(U(1)+U(MPSI))/2.0                                          MAIN      277
                      DO 47 I=2,MPSI                                                 MAIN      278
                      IF ((RD-U(I))*(RD-U(I-1))) 48,48,47                            MAIN      279
                   47 CONTINUE                                                       MAIN      280
          280      48 RHALVE=ETA(I-1)+(ETA(I)-ETA(I-1))*(RD-U(I-1))/(U(I)-U(I-1))    MAIN      281
                      DUMMY=XK2*RHALVE*ABS(U(I)-U(MPSI))*0.025                       MAIN      282
                      XMU(1)=DUMMY*RHO(1)                                            MAIN      283
                      DO 79 I=2,MPSI                                                 MAIN      284
                C     MODEL 2 BEFORE MIXING ZONE REACHES AXIS                        MAIN      285
          285      79 XMU(I)=DUMMY*(RHO(I)*ETA(I)/Y(I))**2/RHO(I)                    MAIN      286
                      GO TO 98                                                       MAIN      287
                C     MODEL 2 AFTER MIXING ZONE REACHES AXIS                         MAIN      288
                   26 RD=(U(1)+U(MPSI))/2.0                                          MAIN      289
                      DO 27 I=2,MPSI                                                 MAIN      290
          290         IF ((RD-U(I))*(RD-U(I-1))) 28,28,27                            MAIN      291
                   27 CONTINUE                                                       MAIN      292
                   28 RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))          MAIN      293
                C     MODEL 3 AFTER MIXING ZONE REACHES AXIS                         MAIN      294
                      XMU(1)=XK2*RHALVE*RHO(1)*ABS(U(1)-U(MPSI))*0.025               MAIN      295
          295         DO 29 I=1,MPSI                                                 MAIN      296
                   29 XMU(I)=XMU(1)                                                  MAIN      297
                      GO TO 98                                                       MAIN      298
                   33 RD=(U(1)+U(MPSI))/2.0                                          MAIN      299
                      DO 34 I=2,MPSI                                                 MAIN      300
          300         IF ((RD-U(I))*(RD-U(I-1))) 35,35,34                            MAIN      301
                   34 CONTINUE                                                       MAIN      302
                   35 RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))          MAIN      303
                C     MODEL 4 AFTER MIXING ZONE REACHES AXIS                         MAIN      304
                      XMU(1)=XK2*RHALVE*RHO(MPSI)*ABS(U(1)-U(MPSI))*0.025            MAIN      305
          305         DO 36 I=1,MPSI                                                 MAIN      306
                   36 XMU(I)=XMU(1)                                                  MAIN      307
                      GO TO 98                                                       MAIN      308
                C      MODEL 5 BEFORE MIXING ZONE REACHES AXIS                       MAIN      309
                 9003 XMU(1) = 0.00137*(X+1.0E-05)*ABS(UNIT-U(MPSI))*RHO(1)          MAIN      310
          310         DO 9004 I = 2,MPSI                                             MAIN      311
                      XMU(I)=0.00137*(X+1.0E-05)*ABS(UNIT-U(MPSI))*(RHO(1)**2/RHO(I))MAIN      312
                 9004 CONTINUE                                                       MAIN      313
                   98 A(1)=0.0                                                       MAIN      314
                C     CALCULATE A                                                    MAIN      315
          315         DO 44 I=2,MPSI                                                 MAIN      316
                   44 A(I)=XMU(I)*RHO(I)*U(I)*Y(I)*Y(I)/PSI(I)                       MAIN      317
                      DO 899 L=1,NPSI                                                MAIN      318
                      RRT=1.986*T(L)                                                 MAIN      319
                      ROOTT=SQRT(T(L))                                               MAIN      320
          320         TX=T(L)                                                        MAIN      321
                      CALL TKEY(TX  ,TTB,ITKEY,SDT,HDT,NT)                          MAIN      322
                      IF (ITKEY.EQ.0) GO TO 9                                        MAIN      323
                      DO 855 I=1,NS                                                  MAIN      324
                      G(I)=0.0                                                       MAIN      325
          325         WP(I)=0.0                                                      MAIN      326
                      WM(I)=0.0                                                      MAIN      327
                      QX(I,L)=0.0                                                    MAIN      328
                      DO 872 J=1,NS                                                  MAIN      329
                  872 CM(I,J,L)=0.0                                                  MAIN      330
          330         CALL LIPLN(ITKEY,I, GTB,SDT,HDT,AX)                            MAIN      331
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                    G(I)=AX                                                    MAIN      332
                  855 CONTINUE                                                 MAIN      333
                C     REACTION CALCULATION                                     MAIN      334
                C     REACTION KINETICS CONTINUE DOWN TO 400 DEGREES K         MAIN      335
      335       C        UNLESS TKINET IS SET TO A VALUE OTHER THAN 400. K     MAIN      336
                C     REACTION KINETICS FOR ALL REACTIONS CONTINUE DOWN TO TKINET MAIN     337
                      IF(T(L)-TKINET) 3256,3256,3259                           MAIN      338
                 3259 CONTINUE                                                 MAIN      339
                      DO 862 I=1,NR                                            MAIN      340
      340             RP(I,L)=0.0                                              MAIN      341
                      RM(I,L)=0.0                                              MAIN      342
                      KK = IRT(I)                                              MAIN      343
                C     REACTION CONSTANT TYPE                                   MAIN      344
                      GO TO (841,842,843,844,845,846,847),KK                   MAIN      345
      345           841 RATE=RC(I,1)*AV                                        MAIN      346
                      GO TO 849                                                MAIN      347
                  842 RATE=RC(I,1)/T(L)*AV                                     MAIN      348
                      GO TO 849                                                MAIN      349
                  843 RATE=RC(I,1)/T(L)/T(L)*AV                                MAIN      350
      350             GO TO 849                                                MAIN      351
                  844 RATE=RC(I,1)/ROOTT*AV                                    MAIN      352
                      GO TO 849                                                MAIN      353
                  845 RATE=RC(I,1)*EXP(RC(I,3)/RRT)*AV                         MAIN      354
                      GO TO 849                                                MAIN      355
      355             846 RATE=RC(I,1)*EXP(RC(I,3)/RRT)/T(L)*AV                MAIN      356
                      GO TO 849                                                MAIN      357
                  847 RATE=RC(I,1)/T(L)/ROOTT*AV                               MAIN      358
                  849 CONTINUE                                                 MAIN      359
                      K=IRR(I)                                                 MAIN      360
      360           C     TYPE OF REACTION                                     MAIN      361
                      GO TO(864,865,866,870,871,834,835,836,837,838),K         MAIN      362
                  870 J1=IRRR(I,1)                                             MAIN      363
                      J2=IRRR(I,2)                                             MAIN      364
                      J3=IRRR(I,3)                                             MAIN      365
      365             E = (G(J1)+G(J2)-G(J3))/RRT                              MAIN      366
                      IF(ABS(E).LT.80.0) GO TO 700                             MAIN      367
                      IF(E.LT.0.0) E= EXP(-80.0)                               MAIN      368
                      IF(E.GT.0.0) E = EXP(80.0)                               MAIN      369
                      GO TO 701                                                MAIN      370
      370           700   E = EXP(E)                                           MAIN      371
                    701   CONTINUE                                             MAIN      372
                       CRR=RATE*RHOOUT(L)                                      MAIN      373
                      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)            MAIN      374
                      RM(I,L)=CRR*ALPHA(J3,L)/E/R/T(L)                         MAIN      375
      375             DO 771 J=1, 3                                            MAIN      376
                      SIGN=1.0                                                 MAIN      377
                      IF (J.GT.2) SIGN=-1.0                                    MAIN      378
                      IROW= IRRR(I,J)                                          MAIN      379
                      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)   MAIN      380
      380             CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)   MAIN      381
                      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)   MAIN      382
                   771 QX(IROW,L)= QX(IROW,L)+ SIGN*RP(I,L)                    MAIN      383
                      GO TO 868                                                MAIN      384
                   871 J1=IRRR(I,1)                                            MAIN      385
      385             J2=25                                                    MAIN      386
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```
                      J3=IRRR(I,3)                                              MAIN      387
                      J4=IRRR(I,4)                                              MAIN      388
                      E = (G(J1)-G(J3)-G(J4))/RRT                               MAIN      389
                      IF( ABS(E).LT.80.0) GO TO 702                             MAIN      390
  390                 IF( E.LT.0.0) E = EXP(-80.0)                              MAIN      391
                      IF( E.GT.0.0) E = EXP(80.0)                               MAIN      392
                      GO TO 703                                                 MAIN      393
                  702 E = EXP(E)                                                MAIN      394
                  703 CONTINUE                                                  MAIN      395
  395                  CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)                    MAIN      396
                      RP(I,L)=CRR*ALPHA(J1,L)                                   MAIN      397
                      RM(I,L)=CRR*R*T(L)*RHOOUT(L)*ALPHA(J3,L)*ALPHA(J4,L)/E    MAIN      398
                      DO 772 J=1, 4                                             MAIN      399
                      SIGN=1.0                                                  MAIN      400
  400                 IF (J.GT.2) SIGN=-1.0                                     MAIN      401
                      IROW= IRRR(I,J)                                           MAIN      402
                      IF(J.EQ.2) IROW=25                                        MAIN      403
                      CM(IROW,J1,L)= CM(IROW,J1,L)+SIGN*CRR                     MAIN      404
                      CM(IROW,J3,L)= CM(IROW,J3,L)-SIGN*RM(I,L)/ALPHA(J3,L)     MAIN      405
  405                 CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)     MAIN      406
                  772 QX(IROW,L)= QX(IROW,L)- SIGN*RM(I,L)                      MAIN      407
                      GO TO 867                                                 MAIN      408
                  864 J1=IRRR(I,1)                                              MAIN      409
                      J2=IRRR(I,2)                                              MAIN      410
  410                 J3=IRRR(I,3)                                              MAIN      411
                      J4=IRRR(I,4)                                              MAIN      412
                      E = (G(J1)+G(J2)-G(J3)-G(J4))/RRT                         MAIN      413
                      IF(ABS(E).LT.80.0) GO TO 704                              MAIN      414
                      IF(E.LT.0.0) E = EXP(-80.0)                               MAIN      415
  415                 IF(E.GT.0.0) E = EXP(80.0)                                MAIN      416
                      GO TO 705                                                 MAIN      417
                  704 E = EXP(E)                                                MAIN      418
                  705 CONTINUE                                                  MAIN      419
                       CRR=RATE*RHOOUT(L)*RHOOUT(L)                             MAIN      420
  420                 RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                       MAIN      421
                      RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)/E                     MAIN      422
                      DO 773 J=1,  4                                            MAIN      423
                      SIGN=1.0                                                  MAIN      424
                      IF (J.GT.2) SIGN=-1.0                                     MAIN      425
  425                 IROW= IRRR(I,J)                                           MAIN      426
                      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)    MAIN      427
                      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)    MAIN      428
                      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)    MAIN      429
                      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)     MAIN      430
  430             773 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-RM(I,L))            MAIN      431
                      GO TO 867                                                 MAIN      432
                  865 J1=IRRR(I,1)                                              MAIN      433
                      J2=IRRR(I,2)                                              MAIN      434
                      J3=IRRR(I,3)                                              MAIN      435
  435                 E = (G(J1)+G(J2)-G(J3))/RRT                               MAIN      436
                      IF(ABS(E).LT.80.0) GO TO 706                              MAIN      437
                      IF(E.LT.0.0) E=EXP(-80.0)                                 MAIN      438
                      IF(E.GT.0.0) E=EXP(80.0)                                  MAIN      439
                      GO TO 707                                                 MAIN      440
  440             706 E = EXP(E)                                                MAIN      441
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                  707   CONTINUE                                                  MAIN      442
                         CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV                 MAIN      443
                        RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)             MAIN      444
                        RM(I,L)=CRR*ALPHA(J3,L)/(E*R*T(L))                        MAIN      445
    445                 DO 774 J=1,3                                              MAIN      446
                        SIGN=1.0                                                  MAIN      447
                        IF (J.GT.2) SIGN=-1.0                                     MAIN      448
                        IROW= IRRR(I,J)                                           MAIN      449
                        CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)    MAIN      450
    450                 CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)    MAIN      451
                        CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)    MAIN      452
                    774 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L   ))                 MAIN      453
                        GO TO 868                                                 MAIN      454
                    866 J1=IRRR(I,1)                                              MAIN      455
    455                 J2=IRRR(I,2)                                              MAIN      456
                        J3=IRRR(I,3)                                              MAIN      457
                        J4=IRRR(I,4)                                              MAIN      458
                        J5=IRRR(I,5)                                              MAIN      459
                        E = (G(J1)+G(J2)-G(J3)-G(J4)-G(J5))/RRT                   MAIN      460
    460                 IF(ABS(E).LT.80.0) GO TO 708                              MAIN      461
                        IF(E.LT.0.0) E=EXP(-80.0)                                 MAIN      462
                        IF(E.GT.0.0) E = EXP(80.0)                                MAIN      463
                        GO TO 709                                                 MAIN      464
                    708 E = EXP(E)                                                MAIN      465
    465             709 CONTINUE                                                  MAIN      466
                         CRR=RATE*RHOOUT(L)*RHOOUT(L)                             MAIN      467
                        RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                       MAIN      468
                        RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)*ALPHA(J5,L)*RHOOUT(L)*R*T(L)/E MAIN 469
                        DO 775 J=1, 5                                             MAIN      470
    470                 SIGN=1.0                                                  MAIN      471
                        IF (J.GT.2) SIGN=-1.0                                     MAIN      472
                        IROW= IRRR(I,J)                                           MAIN      473
                        CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)    MAIN      474
                        CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)    MAIN      475
    475                 CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)    MAIN      476
                        CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)     MAIN      477
                        CM(IROW,J5,L)= CM(IROW,J5,L)-SIGN*RM(I,L)/ALPHA(J5,L)     MAIN      478
                    775 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-2.*RM(I,L))         MAIN      479
                        GO TO 861                                                 MAIN      480
    480                 J1=IRRR(I,1)                                              MAIN      481
                        J2=IRRR(I,2)                                              MAIN      482
                        J3=IRRR(I,3)                                              MAIN      483
                         CRR=RATE*PHOOUT(L)                                       MAIN      484
                        RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)             MAIN      485
    485                 RM(I,L)=0.0                                               MAIN      486
                        DO 776 J=1, 3                                             MAIN      487
                        SIGN=1.0                                                  MAIN      488
                        IF (J.GT.2) SIGN=-1.0                                     MAIN      489
                        IROW= IRRR(I,J)                                           MAIN      490
    490                 CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)    MAIN      491
                        CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)    MAIN      492
                    776 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)                     MAIN      493
                        GO TO 868                                                 MAIN      494
                    838 J1=IRRR(I,1)                                              MAIN      495
    495                 J2=25                                                     MAIN      496
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                J3=IRRR(I,3)                                                    MAIN      497
                J4=IRRR(I,4)                                                    MAIN      498
                 CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)                          MAIN      499
                RR(I,L)=CRR*ALPHA(J1,L)                                         MAIN      500
    500         RM(I,L)=0.0                                                     MAIN      501
                DO 777 J=1, 4                                                   MAIN      502
                SIGN=1.0                                                        MAIN      503
                IF (J.GT.2) SIGN=-1.0                                           MAIN      504
                IROW= IRRR(I,J)                                                 MAIN      505
    505         IF (J.EQ.2) IROW=25                                             MAIN      506
    777 CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*CRR                                  MAIN      507
                GO TO 867                                                       MAIN      508
    834 J1=IRRR(I,1)                                                            MAIN      509
                J2=IRRR(I,2)                                                    MAIN      510
    510         J3=IRRR(I,3)                                                    MAIN      511
                J4=IRRR(I,4)                                                    MAIN      512
                 CRR=RATE*RHOOUT(L)*RHOOUT(L)                                   MAIN      513
                RR(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                             MAIN      514
                RM(I,L)=0.0                                                     MAIN      515
    515         DO 778 J=1, 4                                                   MAIN      516
                SIGN=1.0                                                        MAIN      517
                IF (J.GT.2) SIGN=-1.0                                           MAIN      518
                IROW= IRRR(I,J)                                                 MAIN      519
                CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RR(I,L)/ALPHA(J1,L)          MAIN      520
    520         CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RR(I,L)/ALPHA(J2,L)          MAIN      521
    778 QX(IROW,L)= QX(IROW,L)+ SIGN* RR(I,L)                                   MAIN      522
                GO TO 867                                                       MAIN      523
    835 J1=IRRR(I,1)                                                            MAIN      524
                J2=IRRR(I,2)                                                    MAIN      525
    525         J3=IRRR(I,3)                                                    MAIN      526
                 CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV                       MAIN      527
                RR(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)                   MAIN      528
                RM(I,L)=0.0                                                     MAIN      529
                DO 779 J=1, 3                                                   MAIN      530
    530         SIGN=1.0                                                        MAIN      531
                IF (J.GT.2) SIGN=-1.0                                           MAIN      532
                IROW= IRRR(I,J)                                                 MAIN      533
                CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RR(I,L)/ALPHA(J1,L)          MAIN      534
                CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RR(I,L)/ALPHA(J2,L)          MAIN      535
    535 779 QX(IROW,L)= QX(IROW,L)+ SIGN* RR(I,L)                               MAIN      536
                GO TO 868                                                       MAIN      537
    836 J1=IRRR(I,1)                                                            MAIN      538
                J2=IRRR(I,2)                                                    MAIN      539
                J3=IRRR(I,3)                                                    MAIN      540
    540         J4=IRRR(I,4)                                                    MAIN      541
                J5=IRRR(I,5)                                                    MAIN      542
                 CRR=RATE*RHOOUT(L)*RHOOUT(L)                                   MAIN      543
                RR(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)                             MAIN      544
                RM(I,L)=0.0                                                     MAIN      545
    545         DO 780 J=1, 5                                                   MAIN      546
                SIGN=1.0                                                        MAIN      547
                IF (J.GT.2) SIGN=-1.0                                           MAIN      548
                IROW= IRRR(I,J)                                                 MAIN      549
                CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RR(I,L)/ALPHA(J1,L)          MAIN      550
    550         CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RR(I,L)/ALPHA(J2,L)          MAIN      551
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                  780 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)                          MAIN      552
                C     CALCULATE WDOT                                                MAIN      553
                  861 WP(J5)=WP(J5)+PP(I,L)                                         MAIN      554
                      WM(J5)=WM(J5)+PM(I,L)                                         MAIN      555
      555         867 WP(J4)=WP(J4)+PP(I,L)                                         MAIN      556
                      WM(J4)=WM(J4)+PM(I,L)                                         MAIN      557
                  868 WP(J3)=WP(J3)+PP(I,L)                                         MAIN      558
                      WM(J3)=WM(J3)+PM(I,L)                                         MAIN      559
                      WP(J2)=WP(J2)+PM(I,L)                                         MAIN      560
      560             WM(J2)=WM(J2)+PP(I,L)                                         MAIN      561
                      WP(J1)=WP(J1)+PM(I,L)                                         MAIN      562
                      WM(J1)=WM(J1)+PP(I,L)                                         MAIN      563
                  862 CONTINUE                                                      MAIN      564
                 3256 CONTINUE                                                      MAIN      565
      565             DO 897 J=1,NS                                                 MAIN      566
                  897 WDOT(J,L)=(WP(J)-WM(J))/RHOOUT(L)/U(L)                        MAIN      567
                  899 CONTINUE                                                      MAIN      568
                      IOUT=IOUT+1                                                   MAIN      569
                      CALL SSWTCH(1,K000FX)                                         MAIN      570
      570              GO TO(62,63),K000FX                                          MAIN      571
                   62 EOUT=RHO(1)*ALPHA(IECC,1)*3.108E23                            MAIN      572
                      PRINT 61,X,T(1),U(1),EOUT,IOUT                                MAIN      573
                   61 FORMAT(3H0X=1PE15.7,3H T=1PE15.7,3H U=1PE15.7,6H E/CC=1PE15.7,7H S MAIN      574
                     1TEPS=15)                                                      MAIN      575
      575            63 IF(IFINIS) 64,69,64                                        MAIN      576
                     64 CALL SSWTCH(3,K000FX)                                       MAIN      577
                         GO TO(66,65),K000FX                                        MAIN      578
                     65 IF(X-XMAX) 67,66,66                                         MAIN      579
                     67 IF(PRNT-PCNT) 69,69,68                                      MAIN      580
      580            68 CONTINUE                                                   MAIN      581
                         GO TO 5                                                    MAIN      582
                     66 IFINIS=2                                                    MAIN      583
                     69 CALL OUTPUT                                                 MAIN      584
                        PCNT=0.0                                                    MAIN      585
      585               IF(IFINIS-1) 5,5,6                                        MAIN      586
                C        CHECK DIFFUSION STEP SIZE                                 MAIN      587
                    5 XD=DELPSI*DELPSI*SIGMA(1)/XMU(1)/XLE(1)/12.0 *FDL             MAIN      588
                      DO 511 I=2,NPSI                                               MAIN      589
                      DUMMY=A(I+1)+A(I-1)+A(I)+A(I)                                 MAIN      590
      590             DUMMY=PSI(I)*DELPSI*DELPSI*SIGMA(I)/XLF(I)/DUMMY/1.5*FDL      MAIN      591
                  511 XD=AMIN1(XD,DUMMY)                                            MAIN      592
                      DX=AMIN1(DX,XD)                                               MAIN      593
                      DO 101 I=2,NPSI                                               MAIN      594
                      EX1=PSI(I)*DELPSI**2/DX                                       MAIN      595
      595             EX11=.5*(A(I)+A(I+1))                                         MAIN      596
                      EX12=.5*(A(I)+A(I-1))                                         MAIN      597
                C     INTEGRATE MOMENTUM EQUATION                                   MAIN      598
                      PU(I)=(EX11*(U(I+1)-U(I))+EX12*(U(I-1)-U(I)))/EX1+U(I)        MAIN      599
                      PU(I)=PU(I)-DX*DPDX/RHO(I)/U(I)                               MAIN      600
      600             EX3=0.0                                                       MAIN      601
                      EX4=0.0                                                       MAIN      602
                      DO 21 J=1,NS                                                  MAIN      603
                      EX3=EX3+H(J,I)*WDOT(J,I)                                      MAIN      604
                   21 EX4=EX4+CP(J,I)*(ALPHA(J,I+1)-ALPHA(J,I-1))                   MAIN      605
      605             EX2=EX1*CPRAR(I)                                              MAIN      606
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      EX5=XLE(I)*A(I)/SIGMA(I)                                          MAIN      607
      EX6=.5*(EX5+XLE(I+1)*A(I+1)/SIGMA(I+1))                           MAIN      608
      EX7=.5*(EX5+XLE(I-1)*A(I-1)/SIGMA(I-1))                           MAIN      609
      EX8=CPBAR(I)*A(I)/SIGMA(I)                                        MAIN      610
  610 EX9=.5*(EX8+CPBAR(I+1)*A(I+1)/SIGMA(I+1))                         MAIN      611
      EX10=.5*(EX8+CPBAR(I-1)*A(I-1)/SIGMA(I-1))                        MAIN      612
      EX14=EX4*EX5/4.0                                                  MAIN      613
C     INTEGRATE ENERGY EQUATION                                         MAIN      614
      RT(I)=(U(I+1)-U(I-1))**2*A(I)/EX2/4.0+DX*DPDX/RHO(I)/CPBAR(I)+T(I) MAIN     615
  615 1+((EX9+EX14)*T(I+1)+(EX10-EX14)*T(I-1)-(EX9+EX10)*T(I))/EX2-EX3*DX MAIN     616
     2/CPBAR(I)                                                         MAIN      617
      RHOUIX=DX/(RHOOUT(I)* U(I))                                       MAIN      618
C     INTEGRATE SPECIES EQUATIONS                                       MAIN      619
      DO 41 J=1,NS                                                      MAIN      620
  620  41 QX1(J)     =(EX6*(ALPHA(J,I+1)-ALPHA(J,I))+EX7*(ALPHA(J,I-1)-ALPHA MAIN     621
     1(J,I))/EX1+ALPHA(J,I)*  QX(J,I)*RHOUIX                            MAIN      622
      DO 781 M=1,NS                                                     MAIN      623
      DO 781 N=1,NS                                                     MAIN      624
      CM1(M,N)= CM(M,N,I)*RHOUIX                                        MAIN      625
  625 IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0                                MAIN      626
  781 CONTINUE                                                          MAIN      627
      CALL SLOP(QX1,CM1,NS)                                             MAIN      628
  785 FORMAT (1H , 2I5)                                                 MAIN      629
      DO 782 J=1, NS                                                    MAIN      630
  630 ALPHA(J,I)= QX1(J)                                                MAIN      631
  101 CONTINUE                                                          MAIN      632
      WRITE(6,786) DX,X                                                 MAIN      633
  786 FORMAT(1H ,1P2E12.5)                                              MAIN      634
      EX3=4.0*XMU(1)*DX/DELPSI/DELPSI                                   MAIN      635
  635 RHOUIX=DX/(RHOOUT(1)* U(1))                                       MAIN      636
C     COMPUTE U AT CENTER LINE                                          MAIN      637
      RU(1)=EX3*(U(2)-U(1))+U(1)-DX*DPDX/RHO(1)/U(1)                    MAIN      638
      EX4=0.0                                                           MAIN      639
      DO 200 J=1,NS                                                     MAIN      640
  640 EX4=EX4+H(J,1)*WDOT(J,1)                                          MAIN      641
      ALPHA(J,MPSI)=ALPHA(J,MPSI)                                       MAIN      642
  200 QX1(J)     =EX3*XLF(1)*(ALPHA(J,2)-ALPHA(J,1))/SIGMA(1)+ALPHA(J,1) MAIN     643
     1+  QX(J,1)*RHOUIX                                                 MAIN      644
      DO 783 M=1,NS                                                     MAIN      645
  645 DO 783 N=1,NS                                                     MAIN      646
      CM1(M,N)= CM(M,N,1)*RHOUIX                                        MAIN      647
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0                                MAIN      648
  783 CONTINUE                                                          MAIN      649
      CALL SLOP(QX1,CM1,NS)                                             MAIN      650
  650 DO 784 J=1, NS                                                    MAIN      651
C     COMPUTE SPECIES AT CENTER LINE                                    MAIN      652
  784 ALPHA(J,1)= QX1(J)                                                MAIN      653
C     CALCULATE TEMP. AT CENTER LINE                                    MAIN      654
      RT(1)=EX3*(T(2)-T(1))/SIGMA(1)+T(1)+DX*DPDX/RHO(1)/CPBAR(1)       MAIN      655
  655 1-EX4*DX/CPBAR(1)                                                 MAIN      656
      RT(MPSI)=T(MPSI)                                                  MAIN      657
      IF(IEDGE) 230,231,230                                             MAIN      658
C     COMPUTE TEMP. AND U AT EDGE                                       MAIN      659
  230 RU(MPSI)=U(MPSI)-DX*DPDX/RHO(MPSI)/U(MPSI)                        MAIN      660
  660 RT(MPSI)=T(MPSI)+DX*DPDX/RHO(MPSI)/CPBAR(MPSI)                    MAIN      661
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                      DO 210 I=MPSI,29                                          MAIN      662
                      RU(I)=RU(MPSI)                                            MAIN      663
                      U(I)=RU(MPSI)                                             MAIN      664
                      RT(I)=RT(MPSI)                                            MAIN      665
      665           210 T(I)=RT(MPSI)                                           MAIN      666
                    231 CONTINUE                                                MAIN      667
                      1 IFINIS=1                                                MAIN      668
                    921 SAVEX=X                                                 MAIN      669
                      SAVEDX=DX                                                 MAIN      670
      670             DO 941 I=1,29                                             MAIN      671
                      SAVEU(I)=U(I)                                             MAIN      672
                      SAVET(I)=T(I)                                             MAIN      673
                      DO 940 J=1,NS                                             MAIN      674
                      SAVEA(J,I)=ALPHA(J,I)                                     MAIN      675
      675           940 CONTINUE                                                MAIN      676
                    941 CONTINUE                                                MAIN      677
                      MINIT = 13                                                MAIN      678
                      MHALF = 25                                                MAIN      679
                      NTEST=MPSI-1                                              MAIN      680
      680             DO 967 I=1,NTEST                                          MAIN      681
                C       CHECK NEGATIVE MOLE FRACTION.                           MAIN      682
                    965 DO 967 J=1,NS                                           MAIN      683
                      IF (RALPHA(J,I)) 995,967,967                              MAIN      684
                    967 CONTINUE                                                MAIN      685
      685             X=X+DX                                                    MAIN      686
                      PCNT=PCNT+DX                                              MAIN      687
                      DX=XD                                                     MAIN      688
                      DO 925 I=1,29                                             MAIN      689
                      DO 926 J=1,NS                                             MAIN      690
      690           926 ALPHA(J,I)=RALPHA(J,I)                                  MAIN      691
                      T(I)=RT(I)                                                MAIN      692
                    925 U(I)=RU(I)                                              MAIN      693
                      GO TO 999                                                 MAIN      694
                    995 IF (DX.LT.DXMIN)  GO TO 8000                            MAIN      695
      695           981 DX=SAVEDX/2.0                                           MAIN      696
                      X=SAVEX                                                   MAIN      697
                      DO 985 I=1,29                                             MAIN      698
                      DO 982 J=1,NS                                             MAIN      699
                    982 ALPHA(J,I)=SAVEA(J,I)                                   MAIN      700
      700             T(I)=SAVET(I)                                             MAIN      701
                    985 U(I)=SAVEU(I)                                           MAIN      702
                      GO TO 2                                                   MAIN      703
                C     IF MPSI .GE.26 ,MPSI IS HALVED                            MAIN      704
                  999 IF(MPSI-MHALF) 1001,1500,1500                             MAIN      705
      705         1001 IF(ABS(U(NPSI)-U(MPSI))/U(MPSI)-.010) 1011,1011,1004     MAIN      706
                 1011 IF(ABS(T(NPSI)-T(MPSI))/T(MPSI)-.050) 1002,1002,1004      MAIN      707
                 1002 CONTINUE                                                  MAIN      708
                      GO TO 2000                                                MAIN      709
                 1004 MPSI=MPSI+1                                               MAIN      710
      710             NPSI=MPSI-1                                               MAIN      711
                      DO 1101 I=MPSI,29                                         MAIN      712
                      SAVEU(I)=U(NPSI)                                          MAIN      713
                      RU(I)=U(NPSI)                                             MAIN      714
                      U(I)=U(NPSI)                                              MAIN      715
                      SAVET(I)=T(NPSI)                                          MAIN      716
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                      T(I)=T(NPSI)                                              MAIN      717
                      RT(I)=T(NPSI)                                             MAIN      718
                      DO 1102 J=1,NS                                            MAIN      719
                      SAVEA(J,I)=ALPHA(J,NPSI)                                  MAIN      720
  720                 ALPHA(J,I)=ALPHA(J,NPSI)                                  MAIN      721
 1102 RALPHA(J,I)=ALPHA(J,NPSI)                                                 MAIN      722
 1101 CONTINUE                                                                  MAIN      723
                      GO TO 2000                                                MAIN      724
 1500 IFINIS=0                                                                  MAIN      725
  725                 DELPSI=DELPSI+DELPSI                                      MAIN      726
                      DO 1600 I=1,MINIT                                         MAIN      727
                      DO 1650 J=1,NS                                            MAIN      728
 1650 ALPHA(J,I)=ALPHA(J,2*I-1)                                                 MAIN      729
                      T(I)=T(2*I-1)                                             MAIN      730
  730 1600 U(I)=U(2*I-1)                                                        MAIN      731
                      MPSI=MINIT                                                MAIN      732
                      NPSI=MPSI-1                                               MAIN      733
                      DO 1700 I=MINIT,29                                        MAIN      734
                      DO 1750 J=1,NS                                            MAIN      735
  735                 ALPHA(J,I)=ALPHA(J,MPSI)                                  MAIN      736
 1750 RALPHA(J,I)=ALPHA(J,MPSI)                                                 MAIN      737
                      T(I)=T(MPSI)                                              MAIN      738
                      RT(I)=T(MPSI)                                             MAIN      739
                      U(I)=U(MPSI)                                              MAIN      740
  740 1700 RU(I)=U(MPSI)                                                        MAIN      741
                      DO 1800 I=2,29                                            MAIN      742
 1800 PSI(I)=PSI(I-1)+DELPSI                                                    MAIN      743
                      ITER=0                                                    MAIN      744
                      ISTEP=0                                                   MAIN      745
  745                 GO TO 2000                                                MAIN      746
 8000 WRITE (6,8001)                                                            MAIN      747
 8001 FORMAT(68H1NEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING         MAIN      748
     1OF STEP SIZE)                                                             MAIN      749
                      IFINIS=2                                                  MAIN      750
  750                 GO TO 69                                                  MAIN      751
 2000 CONTINUE                                                                  MAIN      752
                      CALL TICK(ISECS)                                          MAIN      753
                      IELAPS = ISECS-ISECST                                     MAIN      754
                      IF(IELAPS.LT.0) IELAPS = IDIFFT + ISECS                   MAIN      755
  755                 IF(IELAPS.GE.ILIMIT) GO TO 6                              MAIN      756
                      GO TO 2                                                   MAIN      757
  100 FORMAT(14I5)                                                              MAIN      758
  102 FORMAT(8F10.4)                                                            MAIN      759
  111 FORMAT (7(1PE10.3))                                                       MAIN      760
  760 222 FORMAT(A6,7E10.3)                                                     MAIN      761
  333 FORMAT(12A6)                                                              MAIN      762
  444 FORMAT(A6,1X,A6,8X,A6,1X,A6,1X,A6,7X,I2,I1,E8.2,F4.1,F9.1)                MAIN      763
  555 FORMAT(7(1PE10.3))                                                        MAIN      764
  666 FORMAT(10I5)                                                              MAIN      765
  765 1000 FORMAT(7E10.3)                                                       MAIN      766
 9900 FORMAT (39H1 MIXING REGION INTERSECTS AXIS AT X = 1PE15.7)                MAIN      767
    6 IF(IPUNCH.EQ.0.OR.IPUNCH.EQ.2) GO TO 9                                    MAIN      768
                      PUNCH333,(TITLE(I),I=1,12)                                MAIN      769
                      PUNCH 666,MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIME,IPRESS,NT  MAIN  770
  770                 PUNCH 555,FREQA(1),FREQA(2),FREQA(3),FREQA(4),FREQA(5),FREQA(6)  MAIN  771
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      PUNCH 555,X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2                      MAIN      772
      PUNCH 555, DXMIN, EPL,     PC(1),PC(2),PC(3),PC(4)                MAIN      773
      PUNCH 555,PPUNCH,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET          MAIN      774
      PUNCH  555,(T(I),I=1,MPSI)                                        MAIN      775
      PUNCH  555,(U(I),I=1,MPSI)                                        MAIN      776
775   DO 8 I = 1,MPSI                                                   MAIN      777
      PUNCH  555,(ALPHA(J,I),J=1,NS)                                    MAIN      778
    8 CONTINUE                                                          MAIN      779
    9 CONTINUE                                                          MAIN      780
780   END                                                               MAIN      781
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SUBROUTINE OUTPUT                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE     1

      SUBROUTINE OUTPUT                                                          OUTPUT     2
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),         OUTPUT     3
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),         OUTPUT     4
     2          WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),         OUTPUT     5
     3RU(30),U(30),TITLE(12),XLE(30),XMU(30)          ,G(25),WTMIX(30),         OUTPUT     6
     4RC(40,3),IRRP(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),        OUTPUT     7
     5          IRR(40),EREQ(30),SAVEA(25,30),          PC(4),ZID(5),         OUTPUT     8
     6          ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),       OUTPUT     9
     7T4(30),TFDG(30),IRT(40),RP(40,30),RM(40,30)                               OUTPUT    10
      DIMENSION ISAVE(6), FREQA(6), ALOC(50,6), ATI(6), YATT(50)                 OUTPUT    11
      COMMON  A      , RHO    , Y      , T      , PSI    , RT                   OUTPUT    12
      COMMON  SUM    , AR     , HSTAT  , H      , ALPHA  , RALPHA               OUTPUT    13
      COMMON  CP     , SIGMA           , WTMOLE , CPBAR  , C                    OUTPUT    14
      COMMON  AID    , ETA    , RATIO  , RU     , U      , TITLE                OUTPUT    15
      COMMON  XLE    , XMU    ,        , G      , WTMIX  , WDOT                 OUTPUT    16
      COMMON  SAVEU  , SAVET  , WM     , WP     , RC                            OUTPUT    17
      COMMON           SAVEA  ,          PC     , X      , XMAX                  OUTPUT    18
      COMMON  PRNT   , DXMIN  , DX     , TOL    , DELPSI , RJ                   OUTPUT    19
      COMMON  XK2    , P      , ZID    , FREQ   , ECC    , DPDX                 OUTPUT    20
      COMMON  YOUT   , HOUT   , RHOOUT , IRRP   , IRR    , IFINIS               OUTPUT    21
      COMMON  IPAGE  , NPSI   , MY     , NS     , NR     , IEDGE                OUTPUT    22
      COMMON  ITURB  , IPRESS , NPSI   , ITEST  , ITFR   , IECC                 OUTPUT    23
      COMMON  IPT    , XMUOUT , XLT    , T4     , TFDG   , IOUT                 OUTPUT    24
      COMMON  IOUT1  , IOUT2  , RP     , RM     , ISAVE  , IPUNCH               OUTPUT    25
      COMMON IKINET,NFREQA,ALOC,FREQA,00100,00200,00300,00400                    OUTPUT    26
      DATA ZCO/6HCO    /                                                         OUTPUT    27
      DATA ZCO2/6HCO2   /                                                        OUTPUT    28
      DATA ZH2O/6HH2O   /                                                        OUTPUT    29
      BIG=1.0E30                                                                 OUTPUT    30
      DO 5 I=1, NS                                                               OUTPUT    31
      IF (AID(I).EQ.ZCO )  ICO=I                                                 OUTPUT    32
      IF (AID(I).EQ.ZCO2) ICO2=I                                                 OUTPUT    33
      IF (AID(I).EQ.ZH2O) IH2O=I                                                 OUTPUT    34
    5 CONTINUE                                                                   OUTPUT    35
      IF(IECC) 531,539,531                                                       OUTPUT    36
  531 DO 532 I=1,NPSI                                                            OUTPUT    37
  532 ECC(I)=RHO(I)*ALPHA(IECC,I)*3.108E23                                       OUTPUT    38
  539 DO 10 I=1,NPSI                                                             OUTPUT    39
      YOUT(I)=Y(I)/RJ                                                            OUTPUT    40
      XMUOUT(I)=XMU(I)*32.174                                                    OUTPUT    41
      HOUT(I)=HSTAT(I)/45055.31                                                  OUTPUT    42
      SUM(I)=0.0                                                                 OUTPUT    43
      DO 10 J=1,NS                                                               OUTPUT    44
   10 SUM(I)=SUM(I)+ALPHA(J,I)*WTMOLE(J)                                         OUTPUT    45
      UD=.05*U(1)+.95*U(NPSI)                                                    OUTPUT    46
      DO 83 I=2,NPSI                                                             OUTPUT    47
      IF ((U(I)-UD)*(U(I-1)-UD)) 84,84,83                                        OUTPUT    48
   83 CONTINUE                                                                   OUTPUT    49
   84 VR=(Y(I)-Y(I-1))*(UD-U(I-1))/(U(I)-U(I-1))+Y(I-1)                          OUTPUT    50
      TD=.05*T(1)+.95*T(NPSI)                                                    OUTPUT    51
      DO 85 I=2,NPSI                                                             OUTPUT    52
      IF ((T(I)-TD)*(T(I-1)-TD)) 86,86,85                                        OUTPUT    53
   85 CONTINUE                                                                   OUTPUT    54
   86 TR=(Y(I)-Y(I-1))*(TD-T(I-1))/(T(I)-T(I-1))+Y(I-1)                          OUTPUT    55
      TR=TR/RJ                                                                   OUTPUT    56
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                VR=VR/RJ                                                        OUTPUT     57
                DO 87 J=1,NS                                                    OUTPUT     58
                AR(J)=0.0                                                       OUTPUT     59
                AD=.05*ALPHA(J,1)+.95*ALPHA(J,MPSI)                             OUTPUT     60
60              IF(ALPHA(J,MPSI)) 91,92,91                                      OUTPUT     61
             91 DO 88 I=1,MPSI                                                  OUTPUT     62
                IF(ALPHA(J,I)-AD) 88,88,89                                      OUTPUT     63
             88 CONTINUE                                                        OUTPUT     64
             89 AR(J)=Y(I-1)+(Y(I)-Y(I-1))*(AD-ALPHA(J,I-1))/(ALPHA(J,I)-ALPHA(J,I OUTPUT     65
65             I-1))                                                           OUTPUT     66
                AR(J)=AR(J)/RJ                                                  OUTPUT     67
                GO TO 87                                                        OUTPUT     68
             92 DO 93 I=1,MPSI                                                  OUTPUT     69
                IF(ALPHA(J,I)-AD) 94,93,93                                      OUTPUT     70
70           93 CONTINUE                                                        OUTPUT     71
             94 GO TO 89                                                        OUTPUT     72
             87 CONTINUE                                                        OUTPUT     73
                PCNT=0.0                                                        OUTPUT     74
                IPAGE=IPAGE+1                                                   OUTPUT     75
75              WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE                          OUTPUT     76
                WRITE (6,102)                                                   OUTPUT     77
                XORJ=X/RJ                                                       OUTPUT     78
                POUT=P/2117.0                                                   OUTPUT     79
                DPOUT=DPDX/2117.0                                               OUTPUT     80
80              WRITE(6,103) XORJ,DX,POUT                                       OUTPUT     81
                IF (ITURB-6) 8600,8500,8600                                     OUTPUT     82
           8500 WRITE (6,8555)                                                  OUTPUT     83
                QQ101=QQ100/RJ                                                  OUTPUT     84
                QQ201=QQ200/RJ                                                  OUTPUT     85
85              WRITE (6,8556) QQ101,QQ201,QQ300,QQ400                          OUTPUT     86
           8555 FORMAT(1H0,8X,4HHALF,21X,12HINNER MIXING,17X,11HMACH NUMBER,16X,11 OUTPUT     87
              *HMIXING RATE/7X,10HRADIUS/R  ,16X,15HZONE RADIUS/R  ,14X,14HAT HAL OUTPUT     88
              *F RADIUS,14X,11HCOEFFICIENT)                                     OUTPUT     89
           8556 FORMAT (4X,1PE14.6,1P3E28.6)                                    OUTPUT     90
90         8600 WRITE (6,107)                                                   OUTPUT     91
                WRITE (6,509)                                                   OUTPUT     92
                DO 73 I=1,MPSI                                                  OUTPUT     93
                SS1= 89517.501*WTMIX(I)                                         OUTPUT     94
                SS2= CPBAR(I)/(CPBAR(I)-SS1)                                    OUTPUT     95
95              SS=SQRT(SS2*SS1*T(I))                                           OUTPUT     96
                XMACH= U(I)/SS                                                  OUTPUT     97
                IF(IECC) 71,72,71                                               OUTPUT     98
             71 WRITE (6,207)I,YOUT(I),U(I),T(I),RHOOUT(I),XMACH, HOUT(I), XMUOUT( OUTPUT     99
               I),ECC(I),PSI(I),I                                               OUTPUT    100
100             GO TO 73                                                        OUTPUT    101
             72 WRITE (6,307)I,YOUT(I),U(I),T(I),RHOOUT(I),XMACH, HOUT(I), XMUOUT( OUTPUT    102
               I)       ,PSI(I),I                                              OUTPUT    103
             73 CONTINUE                                                        OUTPUT    104
                DO 581 I=1,MPSI                                                 OUTPUT    105
105             DO 581 J=1,NS                                                   OUTPUT    106
            581 ALPHA(J,I)=ALPHA(J,I)/WTMIX(I)                                  OUTPUT    107
                IRPT=(NS+6)/7                                                   OUTPUT    108
                DO 564 KK=1,IRPT                                                OUTPUT    109
                II=1+(KK-1)*7                                                   OUTPUT    110
110             I2=7+(KK-1)*7                                                   OUTPUT    111
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      SUBROUTINE  OUTPUT                                CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE
                  WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE                                OUTPUT    112
                  WRITE (6,409)                                                         OUTPUT    113
                  WRITE (6,108)(AID(J),J=I1,12)                                         OUTPUT    114
                  DO 81 I=1,MPSI                                                        OUTPUT    115
  115            81 WRITE (6,208)I,YOUT(I),(RALPHA(J,I),J=I1,12),I                      OUTPUT    116
                  IF(IOUT1)564,564,74                                                   OUTPUT    117
                  74 WRITE (6,420)                                                      OUTPUT    118
                  WRITE (6,421)(AID(J),J=I1,12)                                         OUTPUT    119
                  DO 82 I=1,MPSI                                                        OUTPUT    120
  120             IF(T(I)-TKINET) 564,564,82                                            OUTPUT    121
                  82 WRITE (6,422)I,(WDOT(J,I),J=I1,12),I                               OUTPUT    122
                 564 CONTINUE                                                           OUTPUT    123
                  IF(IOUT2)567,567,75                                                   OUTPUT    124
                  75 IPPT=(NR+9)/10                                                     OUTPUT    125
  125             N=0                                                                   OUTPUT    126
                  NNR=NR-1                                                              OUTPUT    127
                  DO 565 KK=1,IRPT                                                      OUTPUT    128
                  I1=0                                                                  OUTPUT    129
                  N=N+1                                                                 OUTPUT    130
  130             WRITE (6,201)X,(TITLE(I),I=1,12),IPAGE                                OUTPUT    131
                  65 I1=1+(N-1)*5                                                       OUTPUT    132
                  I2=5+(N-1)*5                                                          OUTPUT    133
                  NNN1=I1                                                               OUTPUT    134
                  NNN2=I1+1                                                             OUTPUT    135
  135             NNN3=I1+2                                                             OUTPUT    136
                  NNN4=I1+3                                                             OUTPUT    137
                  NNN5=I2                                                               OUTPUT    138
                  WRITE(6,209)                                                          OUTPUT    139
                  WRITE (6,431)NNN1,NNN2,NNN3,NNN4,NNN5                                 OUTPUT    140
  140             WRITE (6,432)                                                         OUTPUT    141
                  DO 63 I=1,MPSI                                                        OUTPUT    142
                  IF(T(I)-TKINET) 566,564,63                                            OUTPUT    143
                  63 WRITE(6,433)I,YOUT(I),(RP(J,I),RM(J,I),J=I1,12),I                  OUTPUT    144
                 566 IF(NNR/(5*N))565,565,64                                            OUTPUT    145
  145             64 IF(LL)565,66,565                                                   OUTPUT    146
                  66 N=N+1                                                              OUTPUT    147
                  LL=1                                                                  OUTPUT    148
                  GO TO 65                                                              OUTPUT    149
                 565 CONTINUE                                                           OUTPUT    150
  150            567 CONTINUE                                                           OUTPUT    151
                  IF(IPUNCH.EQ.0.OR.IPUNCH.EQ.2) GO TO 568                              OUTPUT    152
                  WRITE(7,790) XORJ,BIG                                                 OUTPUT    153
                C**** COMPUTE AND OUTPUT THE COLLISION FREQUENCY                        OUTPUT    154
                  568 IF (NFREQA) 1065, 1045, 1065                                      OUTPUT    155
  155            1045 WRITE(6,600)                                                      OUTPUT    156
                  WRITE(6,601)                                                          OUTPUT    157
                  GO TO 1066                                                            OUTPUT    158
                 1065 CONTINUE                                                          OUTPUT    159
                  WRITE(6,600)                                                          OUTPUT    160
  160             WRITE(6,601)                                                          OUTPUT    161
                  WRITE (6,1013) (FREQA(J), J=1,NFREQA)                                 OUTPUT    162
                  WRITE (6,1068)                                                        OUTPUT    163
                 1066 DO 802 I=1,NPSI                                                   OUTPUT    164
                  FT1 = 1.0/SQRT(T(I))                                                  OUTPUT    165
  165             FT2 = 1.0/FT1                                                         OUTPUT    166
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      FT3 = 1.0/T(I)                                                    OUTPUT   167
      FT4 = T(I)**0.75                                                  OUTPUT   168
      SUMS = 0.0                                                        OUTPUT   169
      DO 603 IDX = 1,6                                                  OUTPUT   170
170   IF(ISAVE(IDX).EQ.0) GO TO 603                                     OUTPUT   171
      K = ISAVE(IDX)                                                    OUTPUT   172
      TERM = RALPHA(K,I)                                                OUTPUT   173
      GO TO (604,605,606,607,608,614),IDX                               OUTPUT   174
 604  Q = (1.29E-17)*FT2 + 2.46E-16                                     OUTPUT   175
175   GO TO 609                                                         OUTPUT   176
 605  Q = (0.758E-13)*FT1                                               OUTPUT   177
      GO TO 609                                                         OUTPUT   178
 606  Q = (1.53E-11)*FT3                                                OUTPUT   179
      GO TO 609                                                         OUTPUT   180
180   607 Q = (9.0E-18)*FT2 + 8.9E-16                                   OUTPUT   181
      GO TO 609                                                         OUTPUT   182
 608  Q = 3.29E-23*6.21E5*FT2                                           OUTPUT   183
      GO TO 609                                                         OUTPUT   184
 614  Q= 1.85*(6.21)**(-2)*(1.0E-10)*FT3                                OUTPUT   185
185   609 SUMS = SUMS + Q*TERM                                          OUTPUT   186
 603  CONTINUE                                                          OUTPUT   187
      XNEU = (4.57E27)*SUMS*POUT*FT1                                    OUTPUT   188
      ECON= 0.07157*   ECC(I)/XNEU                                      OUTPUT   189
      IF (NFREQA) 1000, 1001, 1000                                      OUTPUT   190
190  1000 CATT = 1.17                                                   OUTPUT   191
      DO 1003 J = 1,NFREQA                                              OUTPUT   192
      ALOC1 = 1. + (6.283*6.283*FREQA(J)*FREQA(J)*1.0E12/(XNEU*XNEU))   OUTPUT   193
 1003 ALOC(I,J) = CATT*ECC(I)/(XNEU*ALOC1)                              OUTPUT   194
      GO TO 1008                                                        OUTPUT   195
195  1001 WRITE(6,610) I, YOUT(I),XNEU ,ECON                           OUTPUT   196
      GO TO 1010                                                        OUTPUT   197
 1008 WRITE(6,610) I, YOUT(I),XNEU,ECON,(ALOC(I,J),J=1,NFREQA)         OUTPUT   198
 1010 IF (IPUNCH.EQ.0.OR.IPUNCH.EQ.2) GO TO 602                         OUTPUT   199
      RPT = YOUT(I)                                                     OUTPUT   200
200   PPCO = RALPHA(ICO ,I)*POUT                                        OUTPUT   201
      PPCO2= RALPHA(ICO2,I)*POUT                                        OUTPUT   202
      PPH2O= RALPHA(IH2O,I)*POUT                                        OUTPUT   203
      WRITE(7,780) RPT,ECC(I),XNEU,T(I),PPCO,PPCO2,PPH2O                OUTPUT   204
 602  CONTINUE                                                          OUTPUT   205
205   IF (NFREQA) 1009, 1015, 1009                                      OUTPUT   206
 1009 DO 1004 J = 1, NFREQA                                             OUTPUT   207
      DO 1005 I = 1, NPSI                                               OUTPUT   208
 1005 YATT(I) =24.0*RJ*ALOC(I,J)                                        OUTPUT   209
      CALL GRATE(ATT(J),YATT,YOUT,NPSI)                                 OUTPUT   210
210   1004 CONTINUE                                                     OUTPUT   211
      WRITE (6,1014)(ATT(J),J=1,NFREQA)                                 OUTPUT   212
 1015 CONTINUE                                                          OUTPUT   213
  102 FORMAT(1H0,8X,3HX/R,                          8X,12HDELTA X      OUTPUT   214
     1FEET,4X,10HPRESS(ATM))                                            OUTPUT   215
215   103 FORMAT(4X,1P6E14.6)                                           OUTPUT   216
  107 FORMAT(4H0 PT,5X,3HY/R, 6X,8HVELOCITY,4X,11HTEMPERATURE,5X,7HDENSI OUTPUT   217
     1TY, 6X,8HMACH NO. , 8X,8HENTHALPY,5X,9HVISCOSITY,5X,*ELECTRON*    OUTPUT   218
     2 ,8X,3HPSI,6X,2HPT )                                              OUTPUT   219
  108 FORMAT(3H0PT,3X,6H Y/R ,7(3X,A6,4X),1X,3H PT)                     OUTPUT   220
220   201 FORMAT(1H1,//////3H X=1PE15.7,5H FEET,8X,12A6,8X,4HPAGE14)    OUTPUT   221
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      SUBROUTINE  OUTPUT                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE   5

                  207 FORMAT(I4,F10.4,1P8E14.6,I4)                                          OUTPUT    222
                  208 FORMAT(I3,F9.5,1P7E13.5,I3)                                           OUTPUT    223
                  209 FORMAT(1H ,//40X,*REACTION RATES (MOLE/ML-SEC)*//)                    OUTPUT    224
                  307 FORMAT(I4,F10.4,1P7E14.6,14X,I4)                                      OUTPUT    225
      225         409 FORMAT(1H0,44X,14HMOLE FRACTIONS)                                     OUTPUT    226
                  420 FORMAT(1H0,35X,36HNET RATE OF PRODUCTION (W-DOT/RHO*U))               OUTPUT    227
                  421 FORMAT(3H0PT,8X,7(3X,A6,4X),1X,3H PT)                                 OUTPUT    228
                  422 FORMAT(I3,9X,1P7E13.5,I3)                                             OUTPUT    229
                  431 FORMAT(1H0,2HPT,4X,3HY/R,8X,5(8HREACTION,I3,11X),2HPT)                OUTPUT    230
      230         432 FORMAT(19X,5(2HRP, 9X,2HRM,10X))                                      OUTPUT    231
                  433 FORMAT(I3,1X,1P11E11.4,I4)                                            OUTPUT    232
                  509 FORMAT(18X,8HFEET/SEC,4X,11H     K      ,6X,5HGM/CC,22X,6HCAL/GM,12  OUTPUT    233
                     1X,9HLB/FT/SEC,3X,*DENSITY(1/ML)*)                                     OUTPUT    234
                  600 FORMAT(1H1,////// 20X,   *COLLISION*, 3X,*ELECTRICAL*,5X,*UNIT ATT   OUTPUT    235
      235            1ENUATION (DB/IN)*/ 20X,*FREQUENCY*,2X,*CONDUCTIVITY*)                 OUTPUT    236
                  601 FORMAT(6H    PT, 7X,3HY/R,5X,*(1/SEC)*, 5X,*(MHO/IN)*/)               OUTPUT    237
                  610 FORMAT(3X,I3,5X,F7.3,8(2X,1PE10.4))                                   OUTPUT    238
                  611 FORMAT(3E15.7)                                                        OUTPUT    239
                  612 FORMAT(E15.7,I5)                                                      OUTPUT    240
      240         780 FORMAT(8(1PE10.3))                                                    OUTPUT    241
                  790 FORMAT(1PE10.3,60X,E10.3)                                             OUTPUT    242
                 1011 FORMAT(1H1,70X,25HLOCAL ATTENUATION (DB/IN))                          OUTPUT    243
                 1012 FORMAT(1H0,19X,9HCOLLISION/20X,9HFREQUENCY/3X,2HPT,16X,7H(1/SEC))     OUTPUT    244
                 1013 FORMAT(19X,25H  SIGN. FREQ. (MEGACYC)= ,6(1PE10.4,2X))               OUTPUT    245
      245        1014 FORMAT(19X,13H   TRANSVERSE/24X,20HATTENUATION (DB) =  ,7(1PE10.4,   OUTPUT    246
                     12X))                                                                  OUTPUT    247
                 1068 FORMAT (1H0)                                                          OUTPUT    248
                 1069 FORMAT (7X,7H(DB/IN))                                                 OUTPUT    249
                      RETURN                                                                OUTPUT    250
      250             END                                                                   OUTPUT    251
```

```
      SUBROUTINE INOUT                                                  INOUT      2
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25), INOUT      3
     1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30), INOUT      4
     2       WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),     INOUT      5
     3RU(30),U(30),TITLE(12),XLE(30),XMU(30)          ,G(25),WTMIX(30),  INOUT      6
     4RC(40,3),IRRR(40,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30), INOUT      7
     5       IRR(40),FREQ(30),SAVEA(25,30),          PC(4),ZID(5),      INOUT      8
     6       ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),   INOUT      9
     7T4(30),TFDG(30),IRT(40),RP(40,30),RM(40,20)                       INOUT     10
      DIMENSION ISAVE(6)                                                INOUT     11
      COMMON  A     , RHO    , Y     , T     , PSI    , RT              INOUT     12
      COMMON  SUM   , AR     , HSTAT , H     , ALPHA  , RALPHA          INOUT     13
      COMMON  CP    , SIGMA  ,       , WTMOLE, CPBAR  , C               INOUT     14
      COMMON  AID   , ETA    , RATIO , RU    , U      , TITLE           INOUT     15
      COMMON  XLE   , XMU    ,       , G     , WTMIX  , WDOT            INOUT     16
      COMMON  SAVEU , SAVET  , WM    , WP    , RC                       INOUT     17
      COMMON         SAVEA   ,       PC    , X      , XMAX            INOUT     18
      COMMON  PRNT  , DXMIN  , DX    , FDL   , DELPSI , RJ              INOUT     19
      COMMON  XK2   , P      , ZID   , FREQ  , ECC    , DPDX            INOUT     20
      COMMON  YOUT  , HOUT   , RHOOUT, IRRP  , IRR    , IFINIS          INOUT     21
      COMMON  IPAGE , MPSI   , MY    , NS    , NR     , IEDGE           INOUT     22
      COMMON  ITURB , IPRESS , NPSI  , ITEST , ITER   , IECC            INOUT     23
      COMMON  IRT   , XMUOUT , XLT   , T4    , TFDG   , IOUT            INOUT     24
      COMMON  IOUT1 , IOUT2  , RP    , RM    , ISAVE  , IPUNCH          INOUT     25
      COMMON TKINET                                                     INOUT     26
      WRITE (6,1901)                                                    INOUT     27
      WRITE (6,1902)                                                    INOUT     28
      WRITE (6,1903)(TITLE(I),I=1,12)                                   INOUT     29
      IF(IPRESS.NE.0) WRITE(6,1904)P                                    INOUT     30
      IF(IPRESS.EQ.0) WRITE(6,1905)P                                    INOUT     31
      WRITE (6,1908)RJ                                                  INOUT     32
      WRITE (6,1909)XLE(1),SIGMA(1)                                     INOUT     33
      WRITE (6,1966)X,XMAX                                              INOUT     34
      WRITE (6,1967)PRNT,DXMIN                                          INOUT     35
      LL=ITURB*2                                                        INOUT     36
      GO TO (1991,1999,1945,1978,1926,1933,9950,8000),LL                INOUT     37
 1991 WRITE (6,1959)                                                    INOUT     38
      GO TO 2999                                                        INOUT     39
 1999 WRITE (6,1960)XK2                                                 INOUT     40
      GO TO 2999                                                        INOUT     41
 1945 WRITE (6,1961)XK2                                                 INOUT     42
      GO TO 2999                                                        INOUT     43
 1978 WRITE (6,1962)XK2                                                 INOUT     44
      GO TO 2999                                                        INOUT     45
 1926 GO TO 2999                                                        INOUT     46
 1933 GO TO 2999                                                        INOUT     47
 8000 WRITE (6,8001)                                                    INOUT     48
 8001 FORMAT(1HU,22X,30HMODIFIED      EDDY VISCOSITY MODEL)             INOUT     49
      GO TO 999                                                         INOUT     50
 9950 WRITE  6,9951)XK2                                                 INOUT     51
 2999 CONTINUE                                                          INOUT     52
      WRITE (6,1916)                                                    INOUT     53
      WRITE (6,1906)T(1),T(MPSI)                                        INOUT     54
      WRITE (6,1907)RT(1),RT(MPSI)                                      INOUT     55
      WTMIX(1)=0.0                                                      INOUT     56
```

```
      WTMIX(MPSI)=0.0                                                    INOUT     57
      DO 1930 J=1,NS                                                     INOUT     58
      WTMIX(1)=WTMIX(1)+ALPHA(J,1)                                       INOUT     59
 1930 WTMIX(MPSI)=WTMIX(MPSI)+ALPHA(J,MPSI)                              INOUT     60
   60 DO 1919 J=1,NS                                                     INOUT     61
      RALPHA(J,1)=ALPHA(J,1)/WTMIX(1)                                    INOUT     62
      RALPHA(J,MPSI)=ALPHA(J,MPSI)/WTMIX(MPSI)                           INOUT     63
 1919 WRITE (6,1917)AID(J),RALPHA(J,1),RALPHA(J,MPSI)                    INOUT     64
      WRITE (6,120)                                                      INOUT     65
   65 DO 159 I=1,NR                                                      INOUT     66
      L=IPR(I)                                                           INOUT     67
      GO TO(131,132,133,134,135,136,137,138,139,140),L                   INOUT     68
  131 J1=IRRR(I,1)                                                       INOUT     69
      J2=IRRR(I,2)                                                       INOUT     70
   70 J3=IRRR(I,3)                                                       INOUT     71
      J4=IRRR(I,4)                                                       INOUT     72
      WRITE (6,121)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)     INOUT     73
      GO TO 159                                                          INOUT     74
  132 J1=IRRR(I,1)                                                       INOUT     75
   75 J2=IRRR(I,2)                                                       INOUT     76
      J3=IRRR(I,3)                                                       INOUT     77
      WRITE (6,122)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)             INOUT     78
      GO TO 159                                                          INOUT     79
  133 J1=IRRR(I,1)                                                       INOUT     80
   80 J2=IRRR(I,2)                                                       INOUT     81
      J3=IRRR(I,3)                                                       INOUT     82
      J4=IRRR(I,4)                                                       INOUT     83
      J5=IRRR(I,5)                                                       INOUT     84
      WRITE (6,123)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J= INOUT     85
   85 1,3)                                                               INOUT     86
      GO TO 159                                                          INOUT     87
  134 J1=IRRR(I,1)                                                       INOUT     88
      J2=IRRR(I,2)                                                       INOUT     89
      J3=IRRR(I,3)                                                       INOUT     90
   90 WRITE (6,124)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)             INOUT     91
      GO TO 159                                                          INOUT     92
  135 J1=IRRR(I,1)                                                       INOUT     93
      J2=IRRR(I,3)                                                       INOUT     94
      J3=IRRR(I,4)                                                       INOUT     95
   95 WRITE (6,125)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)             INOUT     96
      GO TO 159                                                          INOUT     97
  136 J1=IRRR(I,1)                                                       INOUT     98
      J2=IRRR(I,2)                                                       INOUT     99
      J3=IRRR(I,3)                                                       INOUT    100
  100 J4=IRRR(I,4)                                                       INOUT    101
      WRITE (6,126)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)     INOUT    102
      GO TO 159                                                          INOUT    103
  137 J1=IRRR(I,1)                                                       INOUT    104
      J2=IRRR(I,2)                                                       INOUT    105
  105 J3=IRRR(I,3)                                                       INOUT    106
      WRITE (6,127)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)             INOUT    107
      GO TO 159                                                          INOUT    108
  138 J1=IRRR(I,1)                                                       INOUT    109
      J2=IRRR(I,2)                                                       INOUT    110
  110 J3=IRRR(I,3)                                                       INOUT    111
```

```
      J4=IRRR(I,4)                                                      INOUT     112
      J5=IRRR(I,5)                                                      INOUT     113
      WRITE (6,128)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=INOUT     114
     11,3)                                                              INOUT     115
      GO TO 159                                                         INOUT     116
  139 J1=IRRR(I,1)                                                      INOUT     117
      J2=IRRR(I,2)                                                      INOUT     118
      J3=IRRR(I,3)                                                      INOUT     119
      WRITE (6,129)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT     120
      GO TO 159                                                         INOUT     121
  140 J1=IRRR(I,1)                                                      INOUT     122
      J2=IRRR(I,2)                                                      INOUT     123
      J3=IRRR(I,3)                                                      INOUT     124
      WRITE (6,130)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)            INOUT     125
  159 CONTINUE                                                          INOUT     126
  120 FORMAT(1H0,19X,26HREACTIONS BEING CONSIDERED,6X,19HKR=A*EXP(B/RT)/ INOUT     127
     1T**N,7X,1HA,8X,1HN,9X,1HB,7X,*(MOLECULE-ML-SEC UNITS)*)           INOUT     128
  121 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,1PE9.3,2X,0PF4.1,2X INOUT     129
     1,F10.1)                                                           INOUT     130
  122 FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,1PE9.3,2X,0PF4. INOUT     131
     11,2X,F10.1)                                                       INOUT     132
  123 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,10X,1PE9.3,2X,0 INOUT     133
     1PF4.1,2X,F10.1)                                                   INOUT     134
  124 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,1PE9.3,2X,0PF4.1,2X,F10.1)  INOUT     135
  125 FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,1PE9.3,2X,0PF4 INOUT     136
     1.1,2X,F10.1)                                                      INOUT     137
  126 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,1PE9.3,2X,0PF4.1,2X INOUT     138
     1,F10.1,3X,16HONE WAY REACTION)                                    INOUT     139
  127 FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,1PE9.3,2X,0PF4. INOUT     140
     11,2X,F10.1,3X,16HONE WAY REACTION)                                INOUT     141
  128 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,10X,1PE9.3,2X,0 INOUT     142
     1PF4.1,2X,F10.1,3X,16HONE WAY REACTION)                            INOUT     143
  129 FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,1PE9.3,2X,0PF4.1,2X,F10.1,3 INOUT     144
     1X,16HONE WAY REACTION)                                            INOUT     145
  130 FORMAT(I9,9X,A6,2H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,1PE9.3,2X,0PF4 INOUT     146
     1.1,2X,F10.1,3X,16HONE WAY REACTION)                               INOUT     147
 1901 FORMAT(1H1,37X,46HAEROCHEM RESEARCH LABORATORIES  PRINCETON N.J.)  INOUT     148
 1902 FORMAT(25X,*A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUM INOUT     149
     1E PREDICTIONS*)                                                   INOUT     150
 1903 FORMAT(1H0,24X,12A6)                                              INOUT     151
 1904 FORMAT(1H0,22X,19HPRESSURE(INITIAL) =1PE15.7,12H ATMOSPHERES)     INOUT     152
 1905 FORMAT(1H0,22X,20HPRESSURE(CONSTANT) =1PE15.7,12H ATMOSPHERES)    INOUT     153
 1906 FORMAT(23X,24HTEMPERATURE(DEG. KELVIN),3X,1PE15.7,4X,1PE15.7)     INOUT     154
 1907 FORMAT(23X,24HVELOCITY   (FEET/SECOND),3X,1PE15.7,4X,1PE15.7)     INOUT     155
 1908 FORMAT(1H0,22X,14HNOZZLE RADIUS=1PE15.7,5H FEET)                  INOUT     156
 1909 FORMAT(1H0,22X,23HLEWIS NUMBER(CONSTANT)=1PE15.7,5X,25HPRANDTL NUM INOUT     157
     1BER(CONSTANT)=1PE15.7)                                            INOUT     158
 1916 FORMAT(1H0,54X,3HJET,16X,4HEDGE)                                  INOUT     159
 1917 FORMAT(23X,13HMOLE FRACTION,3X,A6,5X,1PE15.7,4X,1PE15.7)          INOUT     160
 1959 FORMAT(1H0,22X,40HLAMINAR VISCOSITY MODEL(SUTHERLANDS LAW))       INOUT     161
 1960 FORMAT(1H0,22X,29HCONSTANT VISCOSITY MODEL  MU=1PE15.7)           INOUT     162
 1961 FORMAT(1H0,22X,27HFERRI VISCOSITY MODEL     K=1PE15.7)           INOUT     163
 1962 FORMAT(1H0,22X,31HTING-LIBBY VISCOSITY MODEL    K=1PE15.7)       INOUT     164
 1966 FORMAT(1H0,22X,14HX INITIAL(FEET)=1PE15.7,12X,14HX FINAL(FEET)=1PE INOUT     165
     115.7)                                                             INOUT     166
```

```
      SUBROUTINE  INOUT                                CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE     4

     1967 FORMAT(1H0,22X,16HPRINT INCREMENT=1PE15.7,12X,18HMINIMUM STEP SIZE INOUT     167
        1=1PE15.7)                                                         INOUT     168
     9951 FORMAT(1H0,22X,69HTING-LIBBY VISCOSITY MODEL AFTER MIXING REGION I INOUT     169
        INTERSECTS X AXIS   K=1PE15.7)                                     INOUT     170
  170   RETURN                                                             INOUT     171
        END                                                                INOUT     172
```

SUBROUTINE GRATE

CDC 6600 FTN V3.0-P312 OPT=2 08/07/72 12.54.49. PAGE 1

```
      SUBROUTINE GRATE(ANSWER,Y,X,N)                                    GRATE   2
      DIMENSION X(30),Y(50)                                             GRATE   3
      SUM = 0.0                                                         GRATE   4
      INTER = N-1                                                       GRATE   5
      I1 = 1                                                            GRATE   6
      I2 = 2                                                            GRATE   7
      DO 1 I = 1,INTER                                                  GRATE   8
      SUM = SUM + (X(I2)-X(I1))*(Y(I2)+Y(I1))                           GRATE   9
      I1 = I1 + 1                                                       GRATE  10
      I2 = I2 + 1                                                       GRATE  11
    1 CONTINUE                                                          GRATE  12
      ANSWER = 0.5*SUM                                                  GRATE  13
      RETURN                                                            GRATE  14
      END                                                               GRATE  15
```

SUBROUTINE TICK

CDC 6600 FTN V3.0-P312 OPT=2 08/07/72 12.54.49. PAGE 1

```
      SUBROUTINE TICK(JJJJ)
      CALL SECOND(TIME)
      JJJJ=TIME
      RETURN
      END
```

```
TICK      2
TICK      3
TICK      4
TICK      5
TICK      6
```

```
      SUBROUTINE SLOP(X,A,N)                                            SLOP      2
C     THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR SLOP      3
C     EQUATIONS BY USING THE GAUSS-GORDAN REDUCTION ALGORITHM WITH THE  SLOP      4
C      DIAGONAL PIVOT STRATEGY                                          SLOP      5
    5 DIMENSION A(25,25),X(25)                                          SLOP      6
      DO 9 K=1,N                                                        SLOP      7
      IF (ABS(A(K,K)) .GT. 1.E-10) GO TO 5                              SLOP      8
      WRITE (6,101)                                                     SLOP      9
      GO TO 99                                                          SLOP     10
   10 5 KP1= K+1                                                        SLOP     11
      DO 6 J= KP1, N                                                    SLOP     12
    6 A(K,J)= A(K,J)/A(K,K)                                             SLOP     13
      X(K)= X(K)/A(K,K)                                                 SLOP     14
      A(K,K)= 1.0                                                       SLOP     15
   15 DO 9 I=1,N                                                        SLOP     16
      IF (I.EQ.K .OR. A(I,K).EQ.0.) GO TO 9                             SLOP     17
      DO 8 J=KP1,N                                                      SLOP     18
    8 A(I,J)= A(I,J)- A(I,K)*A(K,J)                                     SLOP     19
      X(I)= X(I)- A(I,K)*X(K)                                           SLOP     20
   20 A(I,K)=0.                                                         SLOP     21
    9 CONTINUE                                                          SLOP     22
   99 CONTINUE                                                          SLOP     23
  101 FORMAT( * ERROR--- SMALL PIVOT *)                                 SLOP     24
      RETURN                                                            SLOP     25
   25 END                                                               SLOP     26
```

```
 SUBROUTINE  TKEY                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE      1

                SUBROUTINE TKEY(T,TTB,ITKEY,SDT,HDT,NT)                          TKEY       2
                DIMENSION TTB(30)                                                TKEY       3
                NT1=NT-1                                                         TKEY       4
                DO 10 IT=1,NT1                                                   TKEY       5
 5              DT= TTB(IT+1)-TTB(IT)                                            TKEY       6
                SDT=(T-TTB(IT))/DT                                               TKEY       7
                HDT=(TTB(  IT+1)-T) /DT                                          TKEY       8
                IF ((SDT*HDT).GE.0.0) GO TO 11                                   TKEY       9
               10 CONTINUE                                                       TKEY      10
10              WRITE(6,100) T,I                                                 TKEY      11
                ITKEY=0                                                          TKEY      12
              100 FORMAT(1H , *   TEMPERATURE OUT OF RANGE *, E14.5,I5)          TKEY      13
                RETURN                                                           TKEY      14
               11 ITKEY=IT                                                       TKEY      15
15              RETURN                                                           TKEY      16
                END                                                              TKEY      17
```

```
SUBROUTINE LIPLN                    CDC 6600 FTN V3.0-P312 OPT=2  08/07/72  12.54.49.      PAGE      1

      SUBROUTINE LIPLN (ITKEY,I,ATB,SDT,HDT,AX)                          LIPLN      2
      DIMENSION ATB(25,30)                                               LIPLN      3
      AX= ATB(I,ITKEY)*HDT+ ATB(I,ITKEY+1)*SDT                           LIPLN      4
      RETURN                                                             LIPLN      5
5     END                                                                LIPLN      6
```

APPENDIX B

SAMPLE INPUT DATA SHEET

IBM FORTRAN Coding Form

A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

STATEMENT

CARD															
1	SAMPLE TEST CASE														
2	13	17	6	19	1	1	0	60	0	22					
3	9.57	+03													
4	0.0		10.0		1.0		1.0		1.0		0.25		1.0		
5	1.0	-10	2.0												
6	0.1		2000.		300.		7480.		100.				600.		
7, 8, 9	CARD TYPES 7, 8 AND 9 OMITTED														
10.1.1	3.27	-08	5.36	-03	5.04	-02	5.96	-06	5.36	-07	8.14	-02	2.35	-01	
10.1.2	2.35	-01	1.76	-01	2.68	-03	5.16	-07	1.29	-08	6.06	-05	1.19	-03	
10.1.3	1.19	-04	3.40	-02	1.27	-01									
10.2.1	0.0		0.0		0.0		0.0		0.0		0.0		0.0		
10.2.2	0.0		0.0		0.0		0.0		0.0		0.0		0.0		
10.2.3	2.1	-01	0.0		7.9	-01									

IBM

FORTRAN Coding Form

FORTRAN STATEMENT

THERMODYNAMIC DATA CARDS IN THE FOLLOWING ORDER: K, H, HCL, KCL, K^+, H_2, H_2O, CO, CO_2, CL, CL^-, E^-, O, OH, O_2, AL_2O_3, N_2.

11.1.1	K		39.1	21.31						
11.1.2		100.	4.968	42.714	-0.984	200.	4.968	38.751	-0.488	
11.1.3		400.	4.968	38.492	0.506	600.	4.968	39.272	1.500	
11.1.4		800.	4.968	40.084	2.493	1000.	4.968	40.822	3.487	
11.1.5		1200.	4.968	41.481	4.481	1400.	4.970	42.070	5.474	
11.1.6		1600.	4.975	42.602	6.469	1800.	4.988	43.084	7.465	
11.1.7		2000.	5.013	43.526	8.465	2200.	5.057	43.932	9.471	
11.1.8		2400.	5.122	44.310	10.489	2600.	5.213	44.662	11.532	
11.1.9		2800.	5.334	44.993	12.576	3000.	5.489	45.305	13.658	
11.1.10		3200.	5.685	45.601	14.775	3400.	5.932	45.883	15.935	
11.1.11		3600.	6.242	46.153	17.152	3800.	6.630	46.412	18.438	
11.1.12		4000.	7.111	46.664	19.810	4200.	7.701	46.908	21.289	
11.2.1	2ND SPECIES (H)									
:										
11.17.1	18TH SPECIES (N_2)									
:										
11.17.12										

IBM

CHEMICAL REACTION CARDS:

12.1	KCL	+H		=K	+HCL	15	3.0E-11	4072.
12.2	Φ	+Φ	+M	=Φ2	+M	22	1.0E-29	1.0
12.3	H	+H	+M	=H2	+M	22	1.0E-29	1.0
12.4	Φ	+H	+M	=ΦH	+M	22	1.0E-29	1.0
12.5	H	+ΦH	+M	=H2Φ	+M	22	1.0E-28	1.0
12.6	CΦ	+Φ	+M	=CΦ2	+M	26	5.0E-29	1.0 -4000.
12.7	ΦH	+ΦH		=H2Φ	+Φ	15	1.0E-11	-1000.
12.8	ΦH	+H2		=H2Φ	+H	15	4.0E-11	-5500.
12.9	Φ	+H2		=ΦH	+H	15	3.0E-11	-8200.
12.10	H	+Φ2		=ΦH	+Φ	15	3.0E-10	-16500.
12.11	CΦ	+ΦH		=CΦ2	+H	15	5.0E-13	-600.

IBM

FORTRAN Coding Form

FORTRAN STATEMENT

12.12 H	+HCL		=CL	+H2	15	8.8E-11		-4622.
12.13 HCL	+ϕH		=H2ϕ	+CL	15	7.2E-12		-3250.
12.14 ϕH	+CL		=HCL	+ϕ	15	3.0E-11		-5000.
12.15 H	+CL	+M	=HCL	+M	22	3.0E-29		
12.16 K+	+E-	+M	=K	+M	27	2.0E-22	1.5	
12.17 K+	+CL-		=K	+CL	14	1.0E-08	0.5	
12.18 CL	+E-	+M	=CL-	+M	21	3.0E-30		
12.19 H	+CL-		=HCL	+E-	15	1.7E-12		-6210.

APPENDIX C

SAMPLE OUTPUT

AEROCHEM RESEARCH LABORATORIES PRINCETON N.J.
A FAST COMPUTER PROGRAM FOR NONEQUILIBRIUM ROCKET PLUME PREDICTIONS

SAMPLE TEST CASE (8/7/72)

PRESSURE(CONSTANT) = 1.0000000E-01 ATMOSPHERES

NOZZLE RADIUS= 2.5000000E-01 FEET

LEWIS NUMBER(CONSTANT)= 1.0000000E+00 PRANDTL NUMBER(CONSTANT)= 1.0000000E+00

X INITIAL(FEET)= 0. X FINAL(FEET)= 1.0000000E+01

PRINT INCREMENT= 1.0000000E+00 MINIMUM STEP SIZE= 1.0000000E-10

DONALDSON/GRAY VISCOSITY MODEL

		JET	EDGE
TEMPERATURE(DEG. KELVIN)		2.0000000E+03	3.0000000E+02
VELOCITY (FEET/SECOND)		7.4800000E+03	1.0000000E+02
MOLE FRACTION	K	3.2784627E-08	0.
MOLE FRACTION	H	5.3647026E-03	0.
MOLE FRACTION	HCL	5.0467965E-02	0.
MOLE FRACTION	KCL	5.9608140E-06	0.
MOLE FRACTION	K+	5.3647026E-07	0.
MOLE FRACTION	H2	8.1464558E-02	0.
MOLE FRACTION	H2O	2.8512545E-01	0.
MOLE FRACTION	CO	2.3544450E-01	0.
MOLE FRACTION	CO2	1.7683338E-01	0.
MOLE FRACTION	CL	2.6823513E-03	0.
MOLE FRACTION	CL-	5.1659988E-07	0.
MOLE FRACTION	E-	1.2914247E-08	0.
MOLE FRACTION	O	6.0601159E-05	0.
MOLE FRACTION	OH	1.1921228E-03	0.
MOLE FRACTION	O2	1.1921228E-04	2.1000000E-01
MOLE FRACTION	AL2O3	3.4075652E-02	0.
MOLE FRACTION	N2	1.2716243E-01	7.9000000E-01

	REACTIONS BEING CONSIDERED						KP=A*EXP(B/RT)/T**N	A	N	B	(MOLECULE-ML-SEC UNITS)
1	KCL	+ H		= K	+ HCL			3.000E-11	-0.0	4072.0	
2	O	+ O	+ M	= O2	+ M			1.000E-29	1.0	-0.0	
3	H	+ H	+ M	= H2	+ M			1.000E-29	1.0	-0.0	
4	O	+ H	+ M	= OH	+ M			1.000E-29	1.0	-0.0	
5	H	+ OH	+ M	= H2O	+ M			1.000E-28	1.0	-0.0	
6	CO	+ O	+ M	= CO2	+ M			5.000E-29	1.0	-4000.0	
7	OH	+ OH		= H2O	+ O			1.000E-11	-0.0	-1000.0	
8	OH	+ H2		= H2O	+ H			4.000E-11	-0.0	-5500.0	
9	O	+ H2		= OH	+ H			3.000E-11	-0.0	-8200.0	
10	H	+ O2		= OH	+ O			3.000E-10	-0.0	-16500.0	
11	CO	+ OH		= CO2	+ H			5.000E-13	-0.0	-600.0	
12	H	+ HCL		= CL	+ H2			8.800E-11	-0.0	-4622.0	
13	HCL	+ OH		= H2O	+ CL			7.200E-12	-0.0	-3250.0	
14	OH	+ CL		= HCL	+ O			3.000E-11	-0.0	-5000.0	
15	H	+ CL	+ M	= HCL	+ M			3.000E-29	1.0	-0.0	
16	K+	+ E-	+ M	= K	+ M			2.000E-22	1.5	-0.0	
17	K+	+ CL-		= K	+ CL			1.000E-08	.5	-0.0	
18	CL	+ E-	+ M	= CL-	+ M			3.000E-30	-0.0	-0.0	
19	H	+ CL-		= HCL	+ E-			1.700E-12	-0.0	-6210.0	

C-2

X= 0. FEET SAMPLE TEST CASE (8/7/72) PAGE 1

X/R	DELTA x FEET	PRESS(ATM)
0.	2.500000E-02	1.000000E-01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
1.199084E+00	1.019909E+00	1.775436E+00	2.480000E-02

PT	Y/R	VELOCITY FEET/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY LB/FT/SEC	ELECTRON DENSITY(1/ML)	PSI	PT
1	0.0000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	0.	1
2	.1000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.259332E-02	2
3	.2000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	2.518665E-02	3
4	.3000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	3.777997E-02	4
5	.4000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	5.037330E-02	5
6	.5000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	6.296662E-02	6
7	.6000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	7.555994E-02	7
8	.7000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	8.815327E-02	8
9	.8000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.007466E-01	9
10	.9000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.133399E-01	10
11	1.0000	7.480000E+03	2.000000E+03	1.748625E-05	2.723236E+00	-1.239554E+03	4.474016E-03	4.746058E+09	1.259332E-01	11
12	1.3982	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	2.999450E-02	0.	1.385266E-01	12
13	2.2874	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	2.999450E-02	0.	1.511199E-01	13

MOLE FRACTIONS

PT	Y/R	K	H	HCL	KCL	K+	H2	H2O	PT
1	0.00000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	1
2	.10000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	2
3	.20000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	3
4	.30000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	4
5	.40000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	5
6	.50000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	6
7	.60000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	7
8	.70000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	8
9	.80000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	9
10	.90000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	10
11	1.00000	3.27844E-08	5.76470E-03	5.04680E-02	5.96081E-06	5.36470E-07	8.14646E-02	2.85125E-01	11
12	1.39817	0.	0.	0.	0.	0.	0.	0.	12
13	2.28737	0.	0.	0.	0.	0.	0.	0.	13

NET RATE OF PRODUCTION (W=DQT/RHO*U)

PT	K	H	HCL	KCL	K+	H2	H2O	PT
1	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	1
2	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	2
3	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	3
4	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	4
5	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	5
6	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	6
7	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	7
8	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	8
9	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	9
10	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	10
11	3.69229E-04	-1.09439E-04	1.11148E-03	-3.69223E-06	-6.69310E-11	-4.73642E-08	-1.11832E-03	11

X= 0. FEET SAMPLE TEST CASE (8/7/72) PAGE 1

MOLE FRACTIONS

PT	Y/R	CO	CO2	CL	CL-	E-	O	OH	PT
1	0.00000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	1
2	.10000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	2
3	.20000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	3
4	.30000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	4
5	.40000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	5
6	.50000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	6
7	.60000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	7
8	.70000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	8
9	.80000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	9
10	.90000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	10
11	1.00000	2.39449E-01	1.76033E-01	2.68235E-03	5.16600E-07	1.29142E-08	6.06012E-05	1.19212E-03	11
12	1.39817	0.	0.	0.	0.	0.	0.	0.	12
13	2.28737	0.	0.	0.	0.	0.	0.	0.	13

NET RATE OF PRODUCTION (W=DOT/RHO*U)

PT	CO	CO2	CL	CL-	E-	O	OH	PT
1	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	1
2	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	2
3	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	3
4	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	4
5	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	5
6	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	6
7	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	7
8	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	8
9	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	9
10	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	10
11	1.02762E-04	-1.02762E-04	-1.10779E-03	-3.59762E-12	-6.33334E-11	-8.46927E-06	1.23469E-03	11

MOLE FRACTIONS

									PT
1	.00000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	1
	.10000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	2
	.20000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	3
	.30000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	4
	.40000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	5
	.50000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	6
	.60000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	7
	.70000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	8
	.80000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	9
1	.90000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	10
1	1.00000	1.[illegible]E-04	1.40757E-02	1.27162E-01	0.	0.	0.	0.	11
1	[illegible]	2.[illegible]E-01	0.	7.90000E-01	0.	0.	0.	0.	12
1	[illegible]	2.[illegible]E-01	0.	7.90000E-01	0.	0.	0.	0.	13

RATE OF PRODUCTION (W=DOT/PHO*U)

									PT
1		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	1
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	2
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	3
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	4
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	5
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	6
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	7
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	8
		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	9
1		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	10
1		-2.[illegible]E-06	0.	0.	0.	0.	0.	0.	11

XB 0. FEET SAMPLE TEST CASE (8/7/72) PAGE 1

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 1		REACTION 2		REACTION 3		REACTION 4		REACTION 5		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	1
2	1.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	2
3	2.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	3
4	3.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	4
5	4.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	5
6	5.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	6
7	6.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	7
8	7.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	8
9	8.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	9
10	9.0000E-01	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	10
11	1.0000E+00	5.9858E-07	1.1564E-07	1.5093E-12	2.1349E-13	1.1828E-08	8.7195E-10	1.3361E-10	9.4971E-12	2.6284E-08	2.9804E-09	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 6		REACTION 7		REACTION 8		REACTION 9		REACTION 10		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	1
2	1.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	2
3	2.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	3
4	3.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	4
5	4.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	5
6	5.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	6
7	6.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	7
8	7.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	8
9	8.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	9
10	9.0000E-01	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	10
11	1.0000E+00	1.0711E-08	1.1404E-09	2.4730E-06	3.9452E-06	2.1772E-04	3.3490E-04	4.2064E-06	4.0558E-06	6.7424E-07	3.3818E-07	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 11		REACTION 12		REACTION 13		REACTION 14		REACTION 15		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	1
2	1.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	2
3	2.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	3
4	3.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	4
5	4.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	5
6	5.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	6
7	6.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	7
8	7.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	8
9	8.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	9
10	9.0000E-01	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	10
11	1.0000E+00	2.7008E-05	4.0459E-05	1.6657E-03	1.7828E-03	4.2780E-05	7.0427E-05	6.0979E-06	5.9092E-06	1.7742E-08	1.2221E-09	11

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 16		REACTION 17		REACTION 18		REACTION 19		REACTION 20		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	1
2	1.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	2
3	2.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	3
4	3.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	4
5	4.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	5
6	5.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	6
7	6.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	7
8	7.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	8
9	8.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	9
10	9.0000E-01	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	10
11	1.0000E+00	1.2734E-12	4.0314E-14	1.3871E-11	6.3496E-12	8.5421E-12	5.9077E-13	2.2084E-10	2.1994E-10	0.	0.	11

PT	Y/S	CRITICAL FREQUENCY (1/SEC)	ELECTRICAL CONDUCTIVITY (MHO/IN)	UNIT ATTENUATION (DB/IN)
		SIGN. FREQ. (MEGACYC) = 0.7500E+02		
1	0.000	3.0832E+10	1.1017E-02	3.6402E-02
2	.100	3.0832E+10	1.1017E-02	3.6402E-02
3	.200	3.0832E+10	1.1017E-02	3.6402E-02
4	.300	3.0832E+10	1.1017E-02	3.6402E-02
5	.400	3.0832E+10	1.1017E-02	3.6402E-02
6	.500	3.0832E+10	1.1017E-02	3.6402E-02
7	.600	3.0832E+10	1.1017E-02	3.6402E-02
8	.700	3.0832E+10	1.1017E-02	3.6402E-02
9	.800	3.0832E+10	1.1017E-02	3.6402E-02
10	.900	3.0832E+10	1.1017E-02	3.6402E-02
11	1.000	3.0832E+10	1.1017E-02	3.6402E-02
12	1.398	7.3742E+09	0.	0.
		TRANSVERSE ATTENUATION (DB) =		2.6149E-01

2.50000E-02 0.
1.90080E-01 2.50000E-02
2.27558E-01 2.15080E-01
1.77170E-01 4.42638E-01
8.85850E-02 4.42638E-01
1.77170E-01 5.31224E-01
1.27584E-01 7.08394E-01
1.00482E-01 8.35977E-01
9.88847E-02 9.36419E-01

X/R	DELTA X FEET	PRESS(ATM)
4.141214E+00	9.888472E-02	1.000000E-01

HALF RADIUS/R	INNER MIXING ZONE RADIUS/R	MACH NUMBER AT HALF RADIUS	MIXING RATE COEFFICIENT
1.094830E+00	8.188493E-01	1.509756E+00	2.490000E-02

PT	Y/R	VELOCITY FEET/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY LB/FT/SEC	ELECTRON DENSITY(1/ML)	PST	PT
1	0.0000	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907386E-03	4.419308E+09	0.	1
2	.0999	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907386E-03	4.419308E+09	1.259332E-02	2
3	.1998	7.480000E+03	1.995371E+03	1.752709E-05	2.726315E+00	-1.241199E+03	6.907386E-03	4.419308E+09	2.518665E-02	3
4	.2997	7.480000E+03	1.995371E+03	1.752709E-05	2.726314E+00	-1.241199E+03	6.907386E-03	4.419310E+09	3.777997E-02	4
5	.3995	7.479989E+03	1.995371E+03	1.752710E-05	2.726311E+00	-1.241197E+03	6.907389E-03	4.419449E+09	5.037330E-02	5
6	.4994	7.479868E+03	1.995355E+03	1.752724E-05	2.726206E+00	-1.241133E+03	6.907445E-03	4.423511E+09	6.296662E-02	6
7	.5993	7.479279E+03	1.995171E+03	1.752892E-05	2.724674E+00	-1.240205E+03	6.908108E-03	4.484099E+09	7.555994E-02	7
8	.6994	7.477421E+03	1.993991E+03	1.753991E-05	2.711384E+00	-1.232162E+03	6.912437E-03	4.991374E+09	8.815327E-02	8
9	.8007	7.234296E+03	1.969396E+03	1.759384E-05	2.638795E+00	-1.188220E+03	6.929752E-03	7.384200E+09	1.007466E-01	9
10	.9073	6.510506E+03	1.969091E+03	1.777788E-05	2.381637E+00	-1.031756E+03	7.006222E-03	1.317522E+10	1.133399E-01	10
11	1.0310	4.743910E+03	1.827208E+03	1.919058E-05	1.788797E+00	-6.769682E+02	7.562964E-03	1.777640E+10	1.259332E-01	11
12	1.1945	2.300324E+03	1.287576E+03	2.728697E-05	1.014664E+00	-2.773312E+02	1.075373E-02	8.495932E+09	1.385266E-01	12
13	1.4149	9.051555E+02	7.399447E+02	4.751716E-05	5.149041E-01	-9.129333E+01	1.872640E-02	1.356855E+09	1.511199E-01	13
14	1.7194	3.584702E+02	4.491325E+02	7.829308E-05	2.581546E-01	-2.799443E+01	3.085512E-02	9.238785E+08	1.637132E-01	14
15	2.1396	1.659948E+02	3.378280E+02	1.040989E-04	1.372803E-01	-6.838738E+00	4.102512E-02	3.756923E+08	1.763065E-01	15
16	2.6833	1.124715E+02	3.071575E+02	1.144977E-04	9.766968E-02	-9.203940E-01	4.512329E-02	5.995028E+07	1.888999E-01	16
17	3.2422	1.019145E+02	3.010600E+02	1.169176E-04	8.922589E-02	2.905605E-01	4.603755E-02	7.862719E+06	2.014932E-01	17
18	3.7638	1.000003E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	4.620029E-02	0.	2.140865E-01	18
19	4.2521	1.000000E+02	3.000000E+02	1.172305E-04	8.770271E-02	5.116059E-01	4.620029E-02	0.	2.266798E-01	19

MOLE FRACTIONS

PT	Y/R	K	H	HCL	KCL	K+	H2	H2O	PT
1	0.00000	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	1
2	.04988	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	2
3	.14977	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	3
4	.24965	1.56850E-07	5.08545E-03	5.07715E-02	5.83414E-06	5.39186E-07	8.18652E-02	2.84461E-01	4
5	.34953	1.56854E-07	5.08564E-03	5.07714E-02	5.83412E-06	5.39186E-07	8.18647E-02	2.84461E-01	5
6	.44942	1.57035E-07	5.09133E-03	5.07663E-02	5.83368E-06	5.39173E-07	8.18515E-02	2.84457E-01	6
7	.54932	1.59724E-07	5.17653E-03	5.06925E-02	5.82725E-06	5.39012E-07	8.16596E-02	2.84390E-01	7
8	.64941	1.82959E-07	5.91020E-03	5.00578E-02	5.77194E-06	5.37857E-07	8.00444E-02	2.83800E-01	8
9	.80070	2.99167E-07	9.49315E-03	4.67447E-02	5.48223E-06	5.32834E-07	7.20236E-02	2.80084E-01	9
10	.90760	5.91270E-07	1.74667E-02	3.65899E-02	4.57155E-06	5.14889E-07	5.03326E-02	2.61745E-01	10
11	1.03100	8.27781E-07	1.98406E-02	2.89126E-02	2.86265E-06	4.29543E-07	2.28090E-02	2.00135E-01	11
12	1.19652	7.91338E-07	1.11811E-02	6.13179E-03	9.68287E-07	1.96289E-07	6.19345E-03	1.01865E-01	12
13	1.41890	3.88565E-07	3.81455E-03	2.67101E-03	2.63547E-07	6.41387E-08	3.72846E-03	3.62870E-02	13
14	1.71945	8.74038E-08	8.85438E-04	1.17603E-03	1.23100E-07	1.95991E-08	1.65992E-03	1.11777E-02	14
15	2.13955	1.01919E-08	1.51973E-04	7.71461E-04	4.34483E-08	4.87975E-09	5.34077E-04	2.73869E-03	15
16	2.68327	1.26825E-09	1.86231E-05	7.98926E-05	9.08039E-09	9.26440E-10	1.23035E-04	5.07776E-04	16
17	3.36216	1.07638E-10	1.74532E-06	1.28541E-05	1.45620E-09	1.39690E-10	2.06919E-05	7.49219E-05	17
18	3.76375	0.	0.	0.	0.	0.	0.	0.	18
19	4.25210	0.	0.	0.	0.	0.	0.	0.	19

NET RATE OF PRODUCTION (W=DOT/RHO*U)

PT	K	H	HCL	KCL	K+	H2	H2O	PT
1	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	1
2	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	2
3	-6.64882E-11	-5.12473E-07	4.21535E-07	-2.28450E-11	8.93332E-11	5.84653E-06	-5.74394E-06	3
4	-6.64670E-11	-5.12383E-07	4.21486E-07	-2.28665E-11	8.93334E-11	5.84642E-06	-5.74383E-06	4
5	-6.51064E-11	-5.25848E-07	4.17983E-07	-2.42414E-11	8.93498E-11	5.83853E-06	-5.73621E-06	5
6	-3.83322E-11	-3.73239E-07	3.37780E-07	-1.14925E-11	8.98247E-11	5.65207E-06	-5.56658E-06	6
7	2.13294E-10	1.39325E-06	-6.64468E-07	-3.10310E-10	9.70143E-11	3.45840E-06	-3.67145E-06	7
8	1.99602E-09	1.47767E-05	-1.13265E-05	-2.16072E-09	1.64700E-10	-1.37331E-05	1.16571E-05	8
9	1.34543E-08	1.14427E-04	-9.91153E-05	-1.41163E-08	6.62017E-10	-1.46223E-04	1.22852E-04	9
10	4.42172E-08	5.04251E-04	-3.49425E-04	-4.75418E-08	3.32462E-09	-6.62950E-04	4.42510E-04	10
11	5.19314E-08	7.77689E-04	-4.37972E-04	-8.93179E-08	7.38658E-09	-8.44388E-04	5.77806E-04	11
12	-3.45776E-07	-4.12008E-04	-2.82496E-04	3.43164E-07	2.61200E-09	-5.51770E-04	4.59941E-04	12
13	-1.72601E-06	8.85255E-05	-1.88459E-05	1.32608E-06	-6.69097E-11	-5.19879E-05	3.83775E-05	13

MOLE FRACTIONS

PT	Y/R	CO	CO2	CI	CL-	E-	O	OH	PT
1	0.00000	2.353111-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	1
2	.09988	2.353111-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	2
3	.19977	2.353111-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89347E-05	1.70718E-03	3
4	.29965	2.353111-01	1.76973E-01	2.37974E-03	5.20233E-07	1.19973E-08	7.89348E-05	1.70718E-03	4
5	.39953	2.353111-01	1.76973E-01	2.37984E-03	5.20232E-07	1.19977E-08	7.89442E-05	1.70726E-03	5
6	.49942	2.352996-01	1.76967E-01	2.38265E-03	5.20209E-07	1.20086E-08	7.92055E-05	1.70949E-03	6
7	.59932	2.351256-01	1.76895E-01	2.42473E-03	5.19888E-07	1.21720E-08	8.30479E-05	1.74256E-03	7
8	.69941	2.335996-01	1.76322E-01	2.78895E-03	5.17400E-07	1.35410E-08	1.19987E-04	2.03246E-03	8
9	.80070	2.251816-01	1.73470E-01	4.44909E-03	5.06121E-07	1.99862E-08	4.33972E-04	3.63397E-03	9
10	.90726	1.953066-01	1.63158E-01	9.62337E-03	4.73545E-07	3.52964E-08	2.74125E-03	8.84767E-03	10
11	1.03100	1.296956-01	1.30421E-01	1.75220E-02	3.80963E-07	4.41914E-08	9.70302E-03	1.28187E-02	11
12	1.19452	5.930396-02	6.41804E-02	9.78882E-03	1.79322E-07	1.48830E-08	7.78412E-03	3.25615E-03	12
13	1.41890	2.295106-02	2.22697E-02	3.15918E-03	6.20097E-08	1.36597E-09	1.08184E-03	1.52159E-04	13
14	1.71945	7.760356-03	6.76917E-03	6.97186E-04	1.87894E-08	5.64541E-10	2.70964E-04	1.11768E-04	14
15	2.13956	2.049556-03	1.65776E-03	1.06490E-04	4.64453E-09	1.72677E-10	5.03626E-05	3.67502E-05	15
16	2.68327	4.010686-04	3.10788E-04	1.18801E-05	8.89377E-10	2.50529E-11	3.95032E-06	4.26322E-06	16
17	3.24216	6.120126-05	4.63519E-05	1.01155E-06	1.34655E-10	3.22056E-12	9.24337E-08	3.17798E-07	17
18	3.76375	0.	0.	0.	0.	0.	0.	0.	18
19	4.25210	0.	0.	0.	0.	0.	0.	0.	19

NET RATE OF PRODUCTION (W-DOT/RHO*U)

PT	CO	CO2	CI	CL-	E-	O	OH	PT
1	-5.83544E-06	5.83544E-06	-4.21606E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	1
2	-5.83544E-06	5.83544E-06	-4.21606E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	2
3	-5.83544E-06	5.83544E-06	-4.21606E-07	9.39150E-11	-4.58176E-12	-2.46775E-08	-9.42413E-08	3
4	-5.83547E-06	5.83547E-06	-4.21557E-07	9.39150E-11	-4.58157E-12	-2.46762E-08	-9.42855E-08	4
5	-5.83804E-06	5.83808E-06	-4.16052E-07	9.39173E-11	-4.56748E-12	-2.45845E-08	-9.67891E-08	5
6	-5.90629E-06	5.90629E-06	-3.37822E-07	9.40084E-11	-4.18368E-12	-2.26453E-08	-1.35525E-07	6
7	-6.83180E-06	6.83180E-06	6.64682E-07	9.54614E-11	1.55294E-12	-1.65444E-08	-3.02688E-07	7
8	-1.52409E-05	1.52409E-05	1.13286E-05	1.08138E-10	5.65616E-11	-7.56295E-07	7.01983E-07	8
9	-8.39002E-05	8.39002E-05	9.91292E-05	2.75471E-10	3.86545E-10	-1.16830E-05	3.14289E-05	9
10	-4.89032E-04	4.89032E-04	3.49471E-04	1.96081E-09	1.36381E-09	5.23358E-05	2.86055E-04	10
11	-1.22859E-03	1.22859E-03	4.38056E-04	5.15755E-09	2.22902E-09	5.11271E-04	1.93455E-04	11
12	-6.26208E-04	6.26208E-04	2.82150E-04	2.29516E-09	3.16833E-10	1.10596E-03	8.78162E-04	12
13	-4.82731E-05	4.82731E-05	1.75196E-05	2.30802E-10	-2.97712E-10	-8.95360E-05	-4.24589E-05	13

MOLE FRACTIONS

PT	Y/R	O2	AL2O3	N2					PT
1	0.00000	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	1
2	.09988	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	2
3	.19977	1.18409E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	3
4	.29965	1.18411E-04	3.40762E-02	1.27164E-01	0.	0.	0.	0.	4
5	.39953	1.18522E-04	3.40761E-02	1.27165E-01	0.	0.	0.	0.	5
6	.49942	1.21404E-04	3.40747E-02	1.27193E-01	0.	0.	0.	0.	6
7	.59932	1.59615E-04	3.40543E-02	1.27590E-01	0.	0.	0.	0.	7
8	.69941	4.68254E-04	3.38809E-02	1.30968E-01	0.	0.	0.	0.	8
9	.80070	2.20949E-03	3.29493E-02	1.49122E-01	0.	0.	0.	0.	9
10	.90726	1.06917E-02	2.96278E-02	2.13864E-01	0.	0.	0.	0.	10
11	1.03100	4.72881E-02	2.14991E-02	3.72252E-01	0.	0.	0.	0.	11
12	1.19452	1.28105E-01	1.02065E-02	5.91999E-01	0.	0.	0.	0.	12
13	1.41890	1.82567E-01	3.73759E-03	7.17579E-01	0.	0.	0.	0.	13
14	1.71945	2.01611E-01	1.20090E-03	7.66679E-01	0.	0.	0.	0.	14
15	2.11956	2.07954E-01	3.06417E-04	7.84042E-01	0.	0.	0.	0.	15
16	2.68327	2.09424E-01	5.88364E-05	7.88856E-01	0.	0.	0.	0.	16
17	3.24216	2.09945E-01	8.88949E-06	7.89827E-01	0.	0.	0.	0.	17
18	3.76175	2.10000E-01	0.	7.90000E-01	0.	0.	0.	0.	1.
19	4.25210	2.10000E-01	0.	7.90000E-01	0.	0.	0.	0.	19

NET RATE OF PRODUCTION (W=DOT/RHO*U)

PT	O2	AL2O3	N2					PT
1	1.37115E-08	0.	0.	0.	0.	0.	0.	1
2	1.37115E-08	0.	0.	0.	0.	0.	0.	2
3	1.37115E-08	0.	0.	0.	0.	0.	0.	3
4	1.36416E-08	0.	0.	0.	0.	0.	0.	4
5	9.74826E-09	0.	0.	0.	0.	0.	0.	5
6	-9.07719E-08	0.	0.	0.	0.	0.	0.	6
7	-1.42056E-06	0.	0.	0.	0.	0.	0.	7
8	-1.34219E-05	0.	0.	0.	0.	0.	0.	8
9	-1.13249E-04	0.	0.	0.	0.	0.	0.	9
10	-6.74944E-04	0.	0.	0.	0.	0.	0.	10
11	-1.25556E-03	0.	0.	0.	0.	0.	0.	11
12	-1.53513E-03	0.	0.	0.	0.	0.	0.	12
13	2.26721E-05	0.	0.	0.	0.	0.	0.	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/R	REACTION 1		REACTION 2		REACTION 3		REACTION 4		REACTION 5		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	5.5927E-07	5.5927E-07	2.5846E-12	1.9969E-13	1.0728E-08	8.3019E-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	1
2	4.9884E-02	5.5927E-07	5.5927E-07	2.5846E-12	1.9969E-13	1.0728E-08	8.3019E-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	2
3	1.0977E-01	5.5927E-07	5.5927E-07	2.5846F-12	1.9969E-13	1.0728E-08	8.3019F-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	3
4	2.0965E-01	5.5927E-07	5.5927E-07	2.5846F-12	1.9970E-13	1.0728E-08	8.3019F-10	1.6651E-10	1.2902E-11	3.6013E-08	2.7928E-09	4
5	3.0953E-01	5.5929E-07	5.5929E-07	2.5852F-12	1.9988E-13	1.0729E-08	8.3018F-10	1.6654E-10	1.2902E-11	3.6016E-08	2.7928E-09	5
6	4.0942E-01	5.5989E-07	5.5988E-07	2.6024F-12	2.0471E-13	1.0753F-08	8.2989E-10	1.6728E-10	1.2917E-11	3.6105E-08	2.7921E-09	6
7	5.0932F-01	5.6879F-07	5.6874E-07	2.8621F-12	2.6846E-13	1.1120E-08	8.2617F-10	1.7840E-10	1.3139E-11	3.7433F-08	2.7845E-09	7
8	6.0941E-01	6.4439F-07	6.4411E-07	5.9885E-12	7.7520E-13	1.4530E-08	7.9872E-10	2.9498E-10	1.5120E-11	4.9966E-08	2.7345E-09	8
9	8.0070F-01	9.8998F-07	9.8819E-07	7.9065F-11	3.4384E-12	3.7834F-08	6.8095E-10	1.7296F-09	2.5647E-11	1.4483E-07	2.5348E-09	9
10	9.0726F-01	1.5670F-06	1.5615E-06	3.2869F-09	1.2611E-11	1.3345E-07	3.7372E-10	2.0943E-08	4.9318E-11	6.7596E-07	1.7893E-09	10
11	1.0310F+00	1.4034F-06	1.3953E-06	5.5540F-08	6.6849E-12	2.3222E-07	2.6593E-11	1.1357E-07	1.1715E-11	1.5004E-06	1.5975E-10	11
12	1.1945F+00	8.6222F-07	8.8376E-07	1.4497F-07	5.8996E-17	2.9910E-07	1.1884F-16	2.0823E-07	6.2388E-17	8.7105E-07	2.3175E-16	12
13	1.4189E+00	7.8882E-07	8.4585E-07	2.5673F-08	5.2026E-31	3.2002E-07	3.0291F-29	9.0640E-08	2.2203E-30	1.2748E-07	4.0202E-31	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/R	REACTION 6		REACTION 7		REACTION 8		REACTION 9		REACTION 10		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	1.4040F-08	1.0668E-09	5.0921E-06	5.0964E-06	3.1377E-04	3.1443E-04	5.5050E-06	5.5119E-06	6.3167E-07	6.3346E-07	1
2	4.9884F-02	1.4040F-08	1.0668E-09	5.0921F-06	5.0964E-06	3.1377E-04	3.1443E-04	5.5050E-06	5.5119E-06	6.3167E-07	6.3346E-07	2
3	1.0977F-01	1.4040F-08	1.0668E-09	5.0921F-06	5.0964E-06	3.1377E-04	3.1443E-04	5.5050E-06	5.5119E-06	6.3167E-07	6.3346E-07	3
4	2.0965F-01	1.4040F-08	1.0668E-09	5.0921F-06	5.0965E-06	3.1377E-04	3.1443F-04	5.5051E-06	5.5119E-06	6.3168E-07	6.3346E-07	4
5	3.0953F-01	1.4042F-08	1.0668E-09	5.0926F-06	5.0970E-06	3.1378E-04	3.1444E-04	5.5057E-06	5.5124E-06	6.3229E-07	6.3357E-07	5
6	4.0942F-01	1.4088E-08	1.0665E-09	5.1060F-06	5.1137E-06	3.1414E-04	3.1478E-04	5.5230F-06	5.5257E-06	6.4841E-07	6.3650E-07	6
7	5.0932F-01	1.4744F-08	1.0632E-09	5.3063F-06	5.3593E-06	3.1949E-04	3.1988E-04	5.7773E-06	5.7271E-06	8.6655E-07	6.8041E-07	7
8	6.0941E-01	2.1230F-08	1.0416E-09	7.2262F-06	7.7152E-06	3.6540E-04	3.6378E-04	8.1816E-06	7.6288E-06	2.8987E-06	1.1478E-06	8
9	8.0070E-01	7.4591F-08	9.5788E-10	2.3194E-05	2.7376E-05	5.8868E-04	5.7246E-04	2.6622E-05	2.1933E-05	2.1860E-05	7.4539E-06	9
10	9.0726F-01	4.2101F-07	6.6595E-10	1.3997F-04	1.5734E-04	1.0078E-03	9.5259E-04	1.1741E-04	9.8727E-05	1.9029E-04	1.1679E-04	10
11	1.0310F+00	1.2328F-06	5.2719E-11	3.3451E-04	3.4526E-04	6.8894E-04	6.4056E-04	1.8585E-04	1.6742E-04	8.0008E-04	6.8572E-04	11
12	1.1945F+00	1.1565F-06	2.5910E-17	3.8726F-05	3.4390E-05	5.0702E-05	3.3951E-05	3.1625E-05	2.3847E-05	3.6584E-04	2.6934E-04	12
13	1.4189E+00	1.7904F-07	2.1628E-33	1.9171E-07	2.4680E-08	8.7910E-07	2.9288E-08	7.4650E-07	1.9319E-07	4.5483E-06	5.4977E-06	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 11		REACTION 12		REACTION 13		REACTION 14		REACTION 15		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	3.8821E-05	3.8059E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	1
2	9.9884E-02	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	2
3	1.9977E-01	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	3
4	2.9965E-01	3.8821E-05	3.8069E-05	1.5916E-03	1.5915E-03	6.1800E-05	6.1926E-05	7.7607E-06	7.7515E-06	1.5060E-08	1.1655E-09	4
5	3.9953E-01	3.8823E-05	3.8071E-05	1.5916E-03	1.5915E-03	6.1803E-05	6.1928E-05	7.7614E-06	7.7524E-06	1.5061E-08	1.1655E-09	5
6	4.9942E-01	3.8827E-05	3.8111E-05	1.5933E-03	1.5932E-03	6.1878E-05	6.1999E-05	7.7807E-06	7.7773E-06	1.5097E-08	1.1652E-09	6
7	5.9932E-01	3.9602E-05	3.8720E-05	1.6177E-03	1.6176E-03	6.2900E-05	6.3063E-05	8.0719E-06	8.1431E-06	1.5626E-08	1.1610E-09	7
8	6.9941E-01	4.5940E-05	4.3972E-05	1.8247E-03	1.8244E-03	7.2600E-05	7.2262E-05	1.0834E-05	1.1621E-05	2.0569E-08	1.1310E-09	8
9	8.0070E-01	7.9518E-05	6.8919E-05	2.7422E-03	2.7400E-03	1.2155E-04	1.1810E-04	3.2344E-05	3.9291E-05	5.5586E-08	1.0013E-09	9
10	9.0720E-01	1.7113E-04	1.1495E-04	3.9829E-03	3.9859E-03	2.3444E-04	2.2176E-04	1.6423E-04	1.9517E-04	2.2057E-07	6.1725E-10	10
11	1.0310E+00	1.8894E-04	7.8328E-05	2.6217E-03	2.6320E-03	2.0227E-04	1.8880E-04	3.5158E-04	3.8875E-04	4.7460E-07	5.4159E-11	11
12	1.1945E+00	4.1237E-05	3.0862E-06	5.3456E-04	5.4497E-04	2.1781E-05	1.4869E-05	7.3081E-05	9.5069E-05	7.8558E-07	3.0618E-16	12
13	1.4194E+00	1.8981E-08	9.3637E-10	6.3212E-05	6.4365E-05	5.2409E-07	1.7779E-08	7.8507E-07	2.9793E-06	7.9406E-07	7.3814E-20	13

REACTION RATES (MOLE/ML-SEC)

PT	Y/H	REACTION 16		REACTION 17		REACTION 18		REACTION 19		REACTION 20		PT
		RP	RM	RP	RM	RP	RM	RP	RM	RP	RM	
1	0.	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	1
2	9.9884E-02	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	2
3	1.9977E-01	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	3
4	2.9965E-01	1.2014E-12	1.8282E-13	1.4121E-11	2.6851E-11	7.0894E-12	5.6732E-13	2.1103E-10	2.0409E-10	0.	0.	4
5	3.9953E-01	1.2015E-12	1.8282E-13	1.4121E-11	2.6853E-11	7.0900E-12	5.6731E-13	2.1103E-10	2.0409E-10	0.	0.	5
6	4.9942E-01	1.2026E-12	1.8300E-13	1.4120E-11	2.6915E-11	7.1050E-12	5.6720E-13	2.1126E-10	2.0425E-10	0.	0.	6
7	5.9932E-01	1.2191E-12	1.8574E-13	1.4111E-11	2.7456E-11	7.3308E-12	5.6578E-13	2.1467E-10	2.0667E-10	0.	0.	7
8	6.9941E-01	1.3549E-12	2.0986E-13	1.4013E-11	3.6666E-11	9.3970E-12	5.5627E-13	2.4399E-10	2.2662E-10	0.	0.	8
9	8.0070E-01	2.0041E-12	3.2528E-13	1.3676E-11	9.9570E-11	2.3281E-11	5.1891E-13	3.8374E-10	3.1013E-10	0.	0.	9
10	9.0720E-01	3.5828E-12	5.0586E-13	1.2688E-11	4.0057E-10	8.7766E-11	3.9251E-13	6.6346E-10	4.1516E-10	0.	0.	10
11	1.0310E+00	5.2393E-12	1.1266E-13	1.0265E-11	6.8785E-10	1.9323E-10	6.2022E-14	6.2242E-10	2.2120E-10	0.	0.	11
12	1.1945E+00	3.8957E-12	2.0779E-14	5.2976E-12	1.7315E-10	1.3464E-10	2.1972E-18	1.6230E-10	3.8760E-12	0.	0.	12
13	1.4194E+00	1.4130E-12	8.1648E-31	2.3909E-12	9.2604E-13	2.1013E-[illegible]	3.1349E-29	9.6216E-12	5.9951E-16	0.	0.	13

PT	Y/A	COLLISION FREQUENCY (1/SEC)	ELECTRICAL CONDUCTIVITY (MHO/IN)	UNIT ATTENUATION (DB/IN)
		SIG. FREQ. (MEGACYC) =	9.750E+03	
1	0.000	3.0995E+10	1.0241E-02	3.3930E-02
2	.100	3.0995E+10	1.0241E-02	3.3930E-02
3	.200	3.0995E+10	1.0241E-02	3.3930E-02
4	.300	3.0995E+10	1.0241E-02	3.3930E-02
5	.400	3.0995E+10	1.0241E-02	3.3931E-02
6	.499	3.0995E+10	1.0251E-02	3.3962E-02
7	.598	3.0980E+10	1.0393E-02	3.4424E-02
8	.699	3.0928E+10	1.1588E-02	3.8240E-02
9	.801	3.0686E+10	1.7335E-02	5.6254E-02
10	.907	3.0045E+10	3.2445E-02	9.7411E-02
11	1.031	2.8963E+10	4.9231E-02	1.2159E-01
12	1.145	2.3592E+10	2.5773E-02	5.4430E-02
13	1.419	2.0940E+10	4.6375E-03	7.9316E-04
14	1.719	1.6238E+10	4.0595E-03	4.3819E-04
15	2.147	1.0744E+10	2.5026E-03	1.2229E-03
16	2.683	8.1008E+09	5.2965E-04	1.4841E-04
17	3.242	7.4849E+09	7.5163E-05	1.8043E-05
18	3.764	7.3762E+09	0.	0.
		TRANSVERSE ATTENUATION (DB) =		4.5217E-01

8.77292E-02 1.03530E+00
8.34182E-02 1.11903E+00

APPENDIX D

COMPARISON BETWEEN MIXED IMPLICIT/EXPLICIT AND FULLY EXPLICIT FINITE DIFFERENCE SCHEMES

APPENDIX D

Comparisons between rocket exhaust plume calculations obtained using the present program (mixed implicit/explicit scheme) and the original AeroChem program[6] (explicit scheme) have been made in order to (i) demonstrate that both schemes yield identical results and (ii) determine the difference in computer run times between the two schemes. The case investigated is a typical solid propellant exhaust containing potassium as the dominant alkali metal impurity. (Typical input data for such a propellant are given in Appendix B.) The programs were run on a CDC 6600 computer. Comparisons between centerline and radial distributions, velocity, temperature and species mole fractions computed via the mixed implicit/explicit and explicit schemes are shown in Figs. D1-D4. The notation $k_1/100$ means that the rate coefficients for $K + HCl \rightarrow KCl + H$ (which is very near equilibrium, even at a pressure of 0.1 atm) was arbitrarily reduced by a factor of 100. This was necessary in order to run the original (explicit) AeroChem program[6] without excessive computer time. Figures D1-D4 show that the two schemes do, in fact, give identical results and we are therefore confident that the new program properly calculates exhaust plume properties.

The principal advantage of the mixed implicit/explicit scheme over the explicit scheme is that stable integration step sizes are much larger. This is clearly demonstrated via the (typical) step size comparison shown in Fig. D5. Thus even though the computational time for each integration step in the present program is about 4 times greater than in the original AeroChem program (primarily because of the matrix inversion subroutine in the present program) the much larger step sizes still give considerable reductions in computer run time.

Table D-I shows a comparison between computer run times for the present and original programs for a typical solid propellant plume at sea level and at 50 kft. For this case, the original AeroChem program cannot be used (in a practical sense) to compute plume properties--primarily because the reaction $K + HCl \rightarrow KCl + H$ is very nearly in equilibrium--resulting in stable integration step sizes of less than about 10^{-8} ft. Thus we record an (essentially) infinite computer run time in Table D-I. However this case can be run using a modified version of the original AeroChem program[6] which keeps the reaction $K + HCl \rightarrow KCl + H$ identically in equilibrium. Run times are noted to be 30 min and 17 min for the sea level and 50 kft cases, respectively. Using the present program reduces these run times to 2.5 and 2.2 min--a very considerable reduction. If, in addition the program is compiled with the 6600 optimized compiler, the run time then is reduced to 1 min for the 50 kft case.

Additional comparisons (made at AFRPL while demonstrating the present program), between the original and present AeroChem programs for other low altitude plumes also showed reductions in computer run times by factors of from 10 to 30.

TABLE D-I

CDC 6600 COMPUTER RUN TIME, MINUTES

10 ft plume; $r_j = 0.25$ ft

		Sea Level	50 kft
Original AeroChem Program[6]	(Explicit)	∞	∞
Original AeroChem Program[6]	(Explicit-modified to put K + HCl ⇌ KCl + H in equilibrium)	30	17
Present Program	(Mixed Implicit/Explicit)	2.5	2.2
Present Program	(Mixed Implicit/Explicit using CDC 6600 Optimized Compiler)		1.0

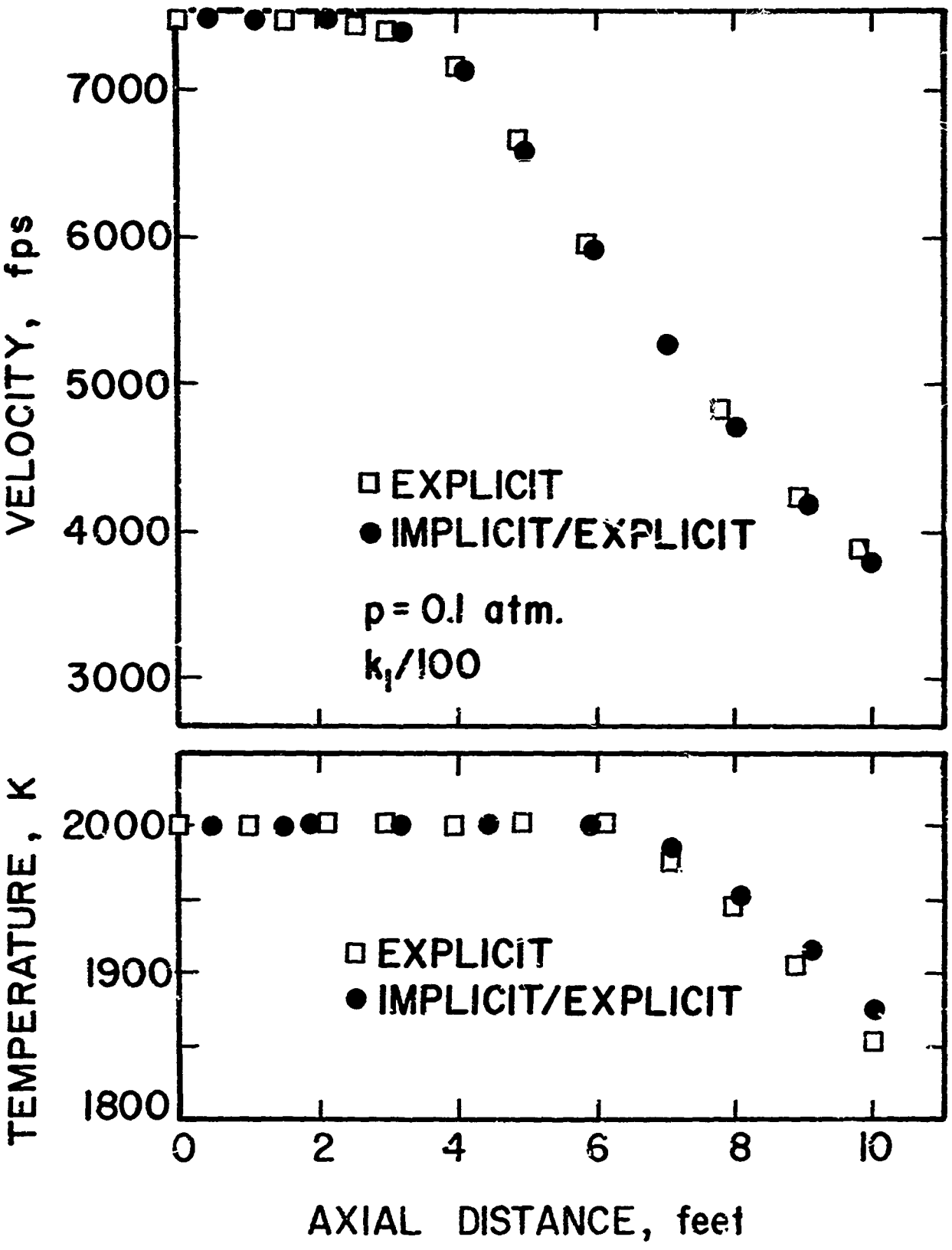

FIG. D1 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

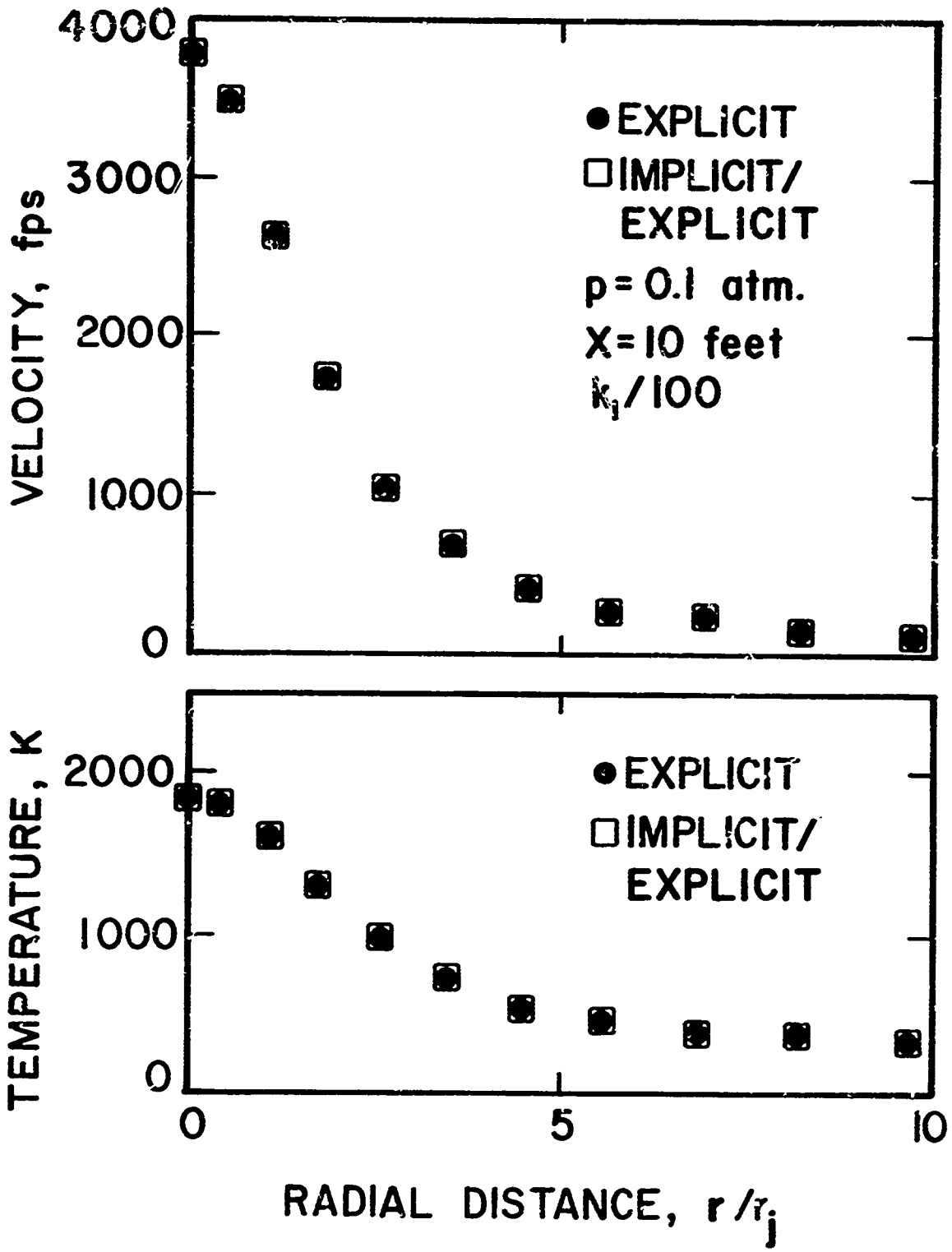

FIG. D2 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF VELOCITY AND TEMPERATURE COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

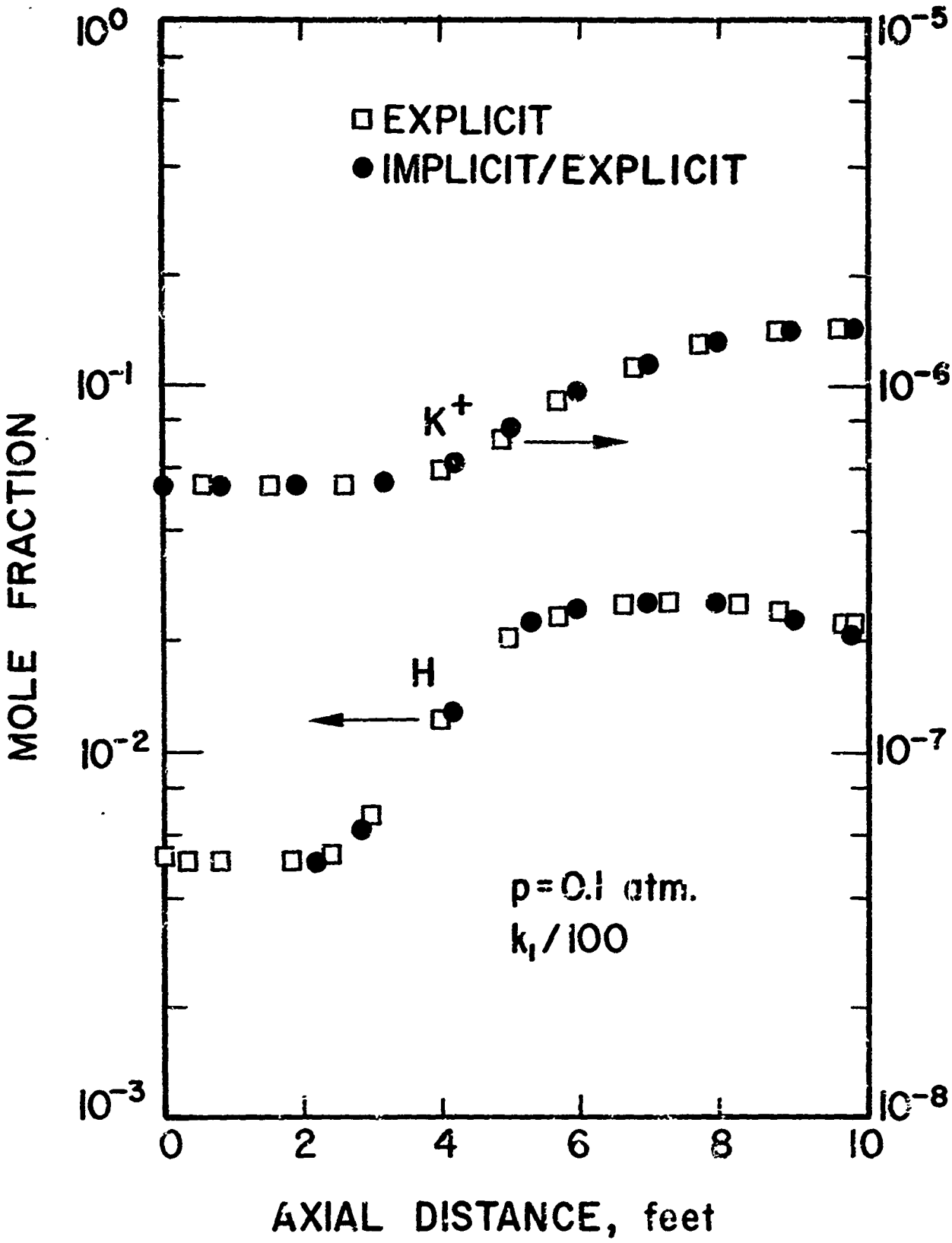

FIG. D3 COMPARISONS BETWEEN CENTERLINE DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

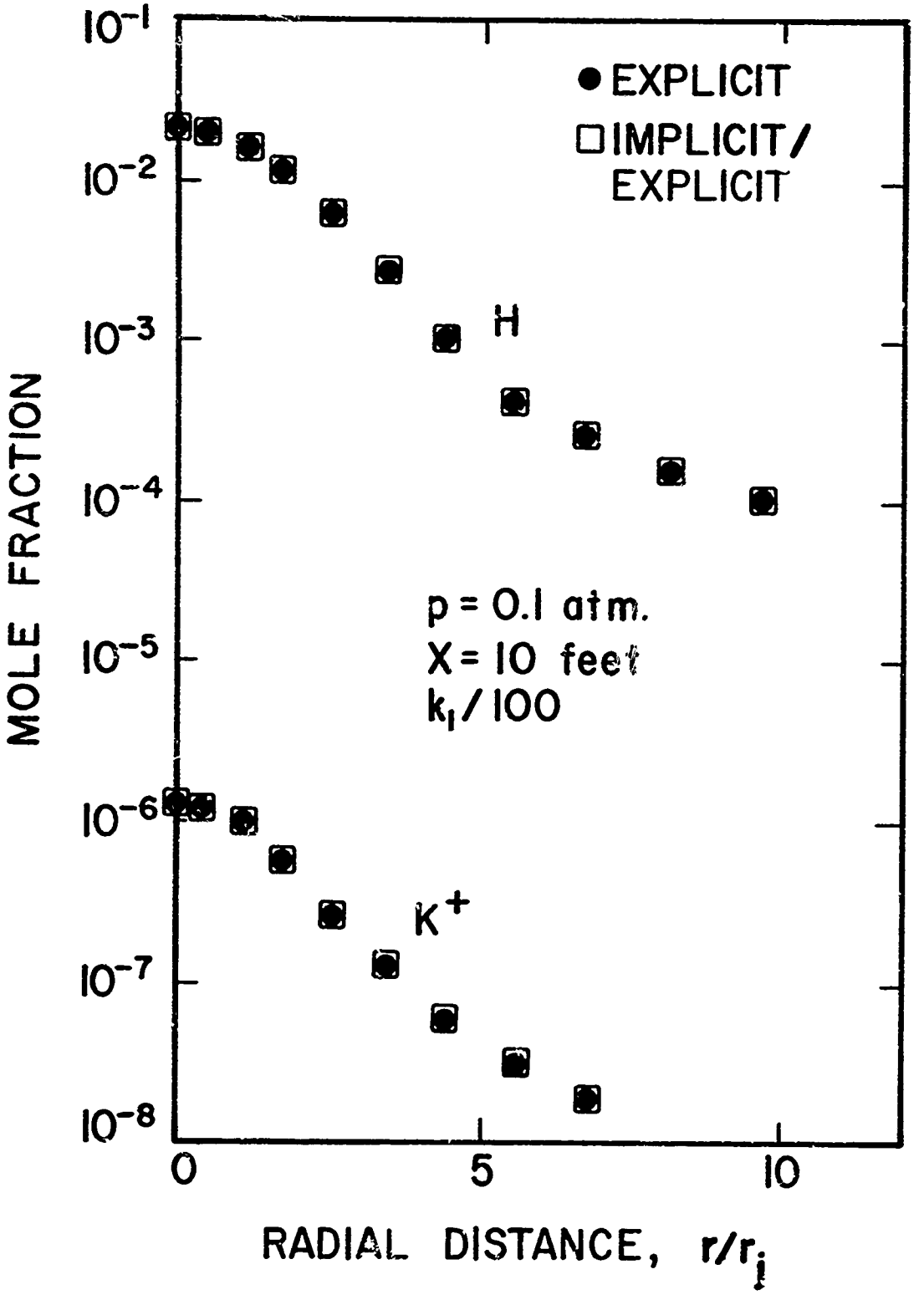

FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft

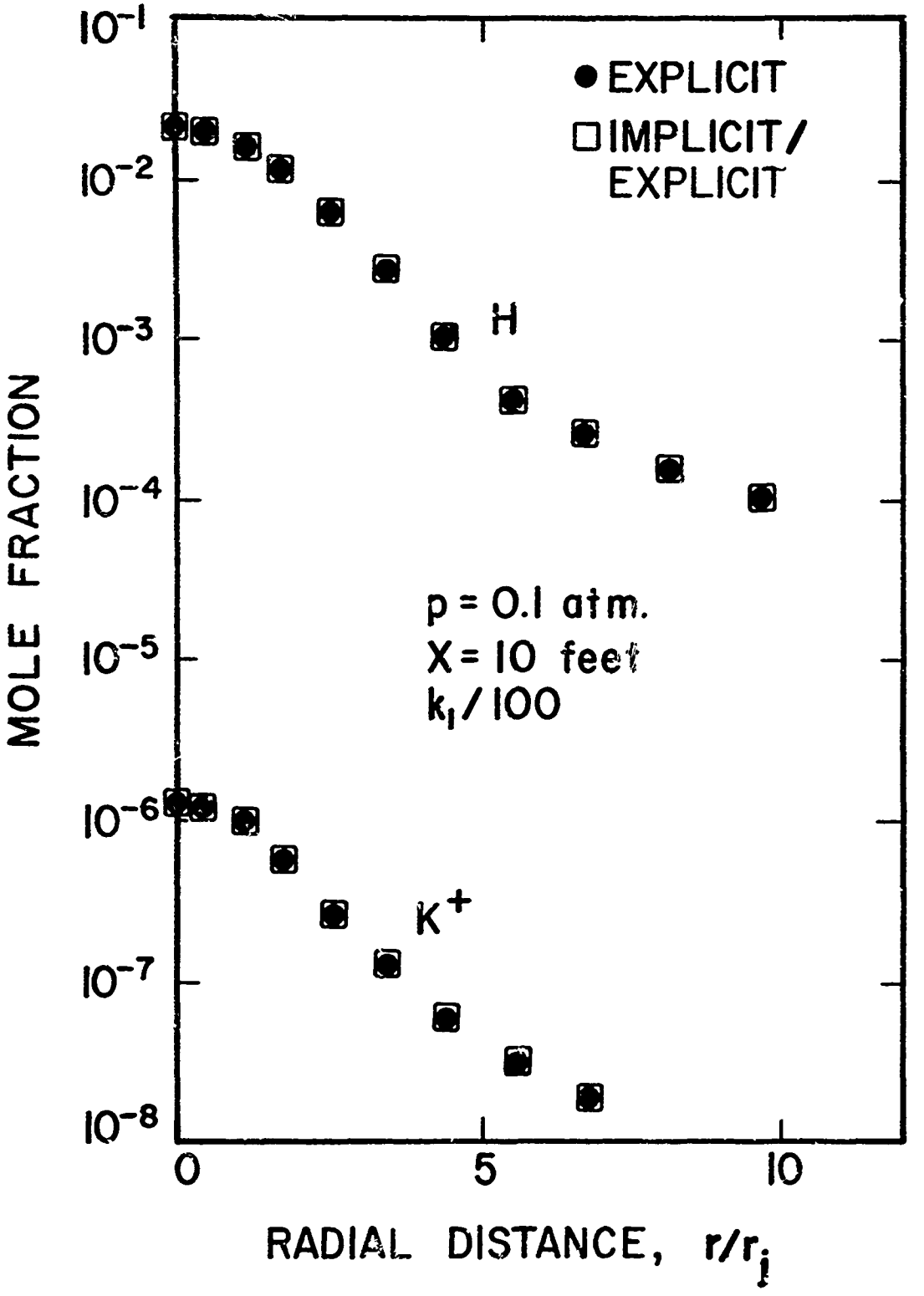

FIG. D4 COMPARISONS BETWEEN RADIAL DISTRIBUTIONS OF X_{K^+} AND X_H COMPUTED FROM MIXED IMPLICIT/EXPLICIT AND EXPLICIT DIFFERENCE TECHNIQUES

$r_j = 0.25$ ft